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Numerical methods for solving the Cahn-Hilliard equation and its applicability to related Energy-based models

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Abstract

In this paper, we review some numerical methods presented in the literature in the last years to approximate the Cahn-Hilliard equation. Our aim is to compare the main properties of each one of the approaches to try to determine which one we should choose depending on which are the crucial aspects when we approximate the equations. Among the properties that we consider desirable to control are the time accuracy order, energy-stability, unique solvability and the linearity or nonlinearity of the resulting systems. In particular, we concern about the iterative methods used to approximate the nonlinear schemes and the constraints that may arise on the physical and computational parameters.

Furthermore, we present the connections of the Cahn-Hilliard equation with other physically motivated systems (not only phase field models) and we state how the ideas of efficient numerical schemes in one topic could be extended to other frameworks in a natural way.

Key words: Cahn-Hilliard, diffuse interface phase-field, energy stability, adaptive time stepping, unique solvability, convergence

1 Introduction

In many scientific, engineering, and industrial applications the study of interfacial dynamics has become the key role to understand the behavior of the systems. For instance, the evolution in time of an interface that separates two materials in the same state arise naturally in hydrodynamics (multi-fluids) while the dynamics of an interface that separates the same material in different states (multi-phases) arise naturally in material science in some processes like solidification or melting. These are some examples but we can find a big amount of applications where

we need to model mixtures of different fluids, solids or gas, due to its connection with many physically motivated problems such as phase separation, Liquid Crystals, Vesicle Membranes deformation, image processing, tumor growth...

These kind of mixtures has been traditionally modeled using sharp interfaces on which a set of interfacial balance conditions must be imposed, arriving at free-boundary models. This kind of approach can be viewed as a system with a *step function* between its properties. It is not a trivial task try to develop a proper notion of generalized solutions for these models and it becomes even more challenging to try to compute numerically the solutions of these systems.

There are several ways of dealing with the computations, but the most conceptually straightforward way of handling the moving interface is to employ a mesh with grid points on the interfaces, that will deform in time according to the equations related with the material on each side of the boundary. Unfortunately, the evolution of the interface may experience topological changes such as self-intersection, pinch-off, splitting, and fattening, and in such a situation this sharp interface formulation breaks down.

To overcome these difficulties, the idea of regularizing the interface considering fixed-grid methods have been highly successful in simulating deforming interfaces. Among these methods we should highlight the volume-of-fluid method, the front-tracking method and the level-set method (for a review of these type of methods we refer the reader to [14]). The main idea of all these approaches consists on representing the interfacial tension as a body force or bulk stress spread over a narrow region covering the interface. Then, over the entire domain we just need to write a single set of governing equations, which can be solved on a fixed grid in a purely Eulerian framework.

An alternative approach for solving interface problems is the *diffuse interface* theory, that is based on describing the dynamic of the interfaces by layers of small thickness and whose structure is determined by a balance of molecular forces, i.e., the tendencies for mixing and de-mixing are in competition through a non-local mixing energy. This idea can be traced to van der Waals [64], and is the foundation for the phase-field theory for phase transition and critical phenomena. One fundamental advantage of these models is that they are able to describe topological transitions like droplet coalescense or droplet break-up in a natural way.

In the *diffuse interface* theory, the surface motion can be derived as the dissipation of a phase-field's free energy functional $E_\varepsilon(\phi)$,

$$\phi_t = -\frac{\delta E_\varepsilon(\phi)}{\delta \phi}$$

where ϕ denotes the so-called phase-field function that is used to localize the phases inside the system, assuming different stable values for each phase (for instance $\phi = 1$ in one phase and $\phi = -1$ in the other one) and over the interfacial regions the function varies smoothly. The width of the interfacial layer depends on a parameter ε appearing in the system. It is interesting

to note that as ε tends to zero the diffuse interface system will converge to the correspondent sharp interface one.

The phase field motion is dictated by a bulk field over the whole domain, and it inherits many interesting properties; ease of coupling with physical variables (velocity and pressure in fluids, temperature, etc.), indifference to morphological singularities in the interface, physical dissipation, and a global space discretization. The value $E_\varepsilon(\phi)$ can represent different interfacial energies associated to the phase field. The most basic energy functional one may introduce is

$$E_\varepsilon(\phi) = \int_\Omega \left(\frac{1}{2}|\nabla\phi|^2 + \frac{1}{\varepsilon^2}F(\phi) \right) dx \tag{1.1}$$

where $F(\phi)$ is a double-well potential to represent the tendency of the system to have two different stable phases and $\varepsilon > 0$ is the parameter related to the interface thickness.

Several choices of the potential $F(\phi)$ can be considered but in this work, we are going to focus on the Ginzburg-Landau double well potential

$$F(\phi) = \frac{1}{4}(\phi^2 - 1)^2 \quad \text{and} \quad f(\phi) = F'(\phi) = (\phi^2 - 1)\phi. \tag{1.2}$$

There are other possible choices of the double well potential like the logarithmic potential F_{log} : $(-1, 1) \to \mathbb{R}$

$$F_{log}(\phi) = \frac{\theta}{2}[(1+\phi)\log(1+\phi) + (1-\phi)\log(1-\phi)] + \frac{\theta_c}{2}(1+\phi)(1-\phi), \tag{1.3}$$

where θ, θ_c are positive constants with $\theta_c > \theta$. It follows that F_{log} has a double-well form with minima at $\pm\beta$ (binodal points) for some $\beta < 1$ (close to 1 in the case of θ_c much larger than θ). The concave region ($F''_{log} < 0$) is an interval $(-\phi_s, \phi_s)$ which is called the spinodal interval. Near $\phi = 0$ this potential leads to the usual approximation of the free energy as quartic polynomial given in (1.2). In contrast with the quartic approximation, the derivatives of F_{log} become unbounded at $\phi = \pm 1$.

The Allen-Cahn and Cahn-Hilliard equations were introduced in [5, 13] to model phase transitions in iron alloys and the thermodynamic forces driving phase separation, respectively. In both cases, the systems are derived as gradient flows

$$\phi_t = -\frac{\delta E(\phi)}{\delta\phi},$$

where $\frac{\delta E(\phi)}{\delta\phi}$ stands for the variational derivative in the $L^2(\Omega)$, $H^{-1}(\Omega)$ norms for Allen-Cahn and Cahn-Hilliard equations, respectively.

As is required by thermodynamics, when there is no external forces we need to ensure that the total "free energy" of the mixture decreases in time. For this purpose we will consider that none of the mixture can pass through the walls of the container, considering as boundary conditions that the outward normal derivatives of ϕ and $\Delta\phi - f(\phi)$ vanish on $\partial\Omega$.

In the Cahn-Hilliard equation, the evolution of the concentration consists of two stages: on the first stage there is a fast phase separation and on the second stage a phase coarsening occurs. At the end of the first stage, fine-scaled phase regions are formed, which are separated by the interface while at the end of the second stage, the solution will reach an equilibrium state, which minimizes the energy functional.

There are three main challenges for solving numerically the Cahn-Hilliard equation; the nonlinearity in the system, the presence of the parameter ε in the equations (which usually is small in phase transition applications) and the different time scales of each of the stages in the evolution of the concentration. Then, an efficient numerical resolution of the problem requires proper relation of numerical scales, that is, the (spatial) mesh size h and the (time) step size k have to properly relate to the interaction length ε.

Two are the main aims of this work: The first one is to review the different numerical approximations of the Cahn-Hilliard model that have been developed in the last years. The second aim consists on showing how interconnected is this system with many physical problems and to show that the ideas from different frameworks can be adapted in a natural way. As a starting point we need to point out that there is no a clear winner in which is the most suitable numerical approximation for the system because all of them have advantages and disadvantages. Our point is that only knowing all the properties of each approach we can compare them to see which one better fulfills with our desires.

Let us now recall the main contributions to the literature in the last years, where there has been an increasing interest in developing efficient and accurate numerical approximations of the Cahn-Hilliard system and many related problems. These models usually deal with two components, but there have been also several extensions where three-phases models have been considered [12, 59, 51, 47, 50] (with and without coupling with a fluid flow).

When the logarithmic potential (1.3) is considered, many authors consider implicit approximations [15, 34] although other nonlinear and energy-stable approaches has been presented in this framework [35].

There are several approximations when the polynomial potential (1.2) is considered. On one hand, implicit approximations (which are not energy-stable, see Definition 2.1 below) have been often considered [24, 25, 26, 31] where a Newton method is usually employed in order to compute the nonlinear scheme. There is an implicit-explicit approximation of the potential that does not introduce any numerical dissipation which have been widely used in phase field models [20, 30, 32, 44, 45] and in the Liquid Crystals context [56]. On the other hand, many authors split the potential into a convex and a non-convex part in order to assure the existence of some numerical dissipation to obtain a unconditional energy-stable scheme [10, 43, 49, 65, 58], although the resulting schemes are nonlinear. These ideas can be traced to Eyre and his celebrated preprint [29]. The idea of splitting the potential has been also considered for thin film

epitaxy [61] where using the approximation that does not introduce dissipation for the convex part and a backward difference scheme in the non-convex part they show that this scheme is energy stable for a perturbed energy.

Trying to circumvent the problem of the nonlinearity and extending Eyre's ideas, some linear (but conditionally energy-stable) schemes have been studied in [63] (which could be unconditionally energy-stable if we introduce large enough numerical dissipation in the system and we truncate the potential term). Moreover, in [6] the authors present one linear and one nonlinear first order in time unconditionally energy-stable schemes in the Nematic Liquid Crystals framework. These schemes are based on the introduction of a Lagrange multiplier in the formulation of the potential term. These ideas were extended by us in [37] where two new linear second order in time approximations of the potential term are derived for the Cahn-Hilliard system. This work is extended in [38], where we study and compare the constraints on the physical and discrete parameters that can appear to assure the energy-stability and unique solvability of these linear schemes with some previous nonlinear schemes, studying also the convergence of Newton's method to the nonlinear schemes. Furthermore, we introduce a new adaptive time step algorithm based on the numerical dissipation introduced in the discrete energy law in each time step. Finally, in the context of tumor growth models, in [67] a linear scheme is presented which is unconditionally energy-stable using a modified formulation of the potential (1.2) and splitting the potential to relax the growth of the potential $F(\phi)$ when $|\phi| > 1$.

Due to the fact of the different time scales that appears in some processes, there have been several attempts [7, 34, 66] to design adaptive time stepping algorithms suitable to be used in the phase field framework where most of them borrow ideas that have been proved successful with Runge-Kutta methods for ODEs.

Among the applications of the understanding and approximating the Cahn-Hilliard equation we should start recalling the coupling between this system with a fluid flow. In [42] the so-called *Model H* was presented which models the mixture of two immiscible, incompressible and viscous Newtonian fluids with the same density. In [40], the authors arrived at the same model from the rational continuum mechanics framework, showing that the system satisfies the second law of thermodynamics, leading in both cases to the so-called Navier-Stokes/Cahn-Hilliard system (NSCH).

There are many works devoted to approximate (NSCH) models that in the most of cases are based on coupling schemes previously presented for Navier-Stokes (see for instance [33]) and Cahn-Hilliard system. Designing models to describe the flow of two immiscible, incompressible and viscous Newtonian fluids with different densities has become a popular and challenging topic in the last years. Indeed, in [57] a thermodynamically consistent extension of the NSCH model with different densities was presented but in this case the velocity field is no longer divergence free, leading to new difficulties to design fully discrete numerical schemes. Recently, the existence

of local in time strong solutions of this system has been studied [2].

In [11], the complete derivation and a numerical approach of a model for the study of incompressible two-fluids mixture with different densities and viscosities was presented, although no energy law of the system is presented.

On the other hand, another model with numerical approximations was introduced in [62] for two-phase incompressible flows with different densities and viscosities.

Finally, in [4] a new thermodynamically consistent model for incompressible two-phase flows with different densities was introduced. Moreover, the existence of weak solutions for this model is proved in [3] and a splitting scheme that segregates the fluid part from the phase field part in a linear and an energy-stable way has been derived in [39]. For a recent review in multi-component mixtures using phase field models we refer the reader to [48]. There is also an increasing interest in more general models that are able to capture the mixture of different complex fluids and we refer the reader to [68] for a formulation using the diffuse-interface method.

This paper is organized as follows. In Section 2 we present the Cahn-Hilliard equation and we recall its main properties and the main analytical results concerning the well posedness of the system. Section 3 is intended to present the different numerical approaches that have been considered for the Cahn-Hilliard equation, reviewing the main properties of each approach. The purpose of Section 4 is to present the connections between the efficient approximations of the Cahn-Hilliard equation with vectorial potentials. In order to do this, we will consider the Nematic Liquid Crystals framework. We first introduce the system and their main analytical aspects and then we present the numerical approaches considered in the literature and the possibility of extending the ideas presented in Section 3. In Section 5 we present two different energy-based models where the ideas of Sections 3 and 4 should be considered to develop efficient numerical schemes. Finally, we state the conclusions of this work in Section 6.

2 Cahn-Hilliard equation

The Cahn-Hilliard equation is a $H^{-1}(\Omega)$ gradient flow of the *Ginzburg-Landau* free energy functional

$$E(\phi) = E_{philic}(\phi) + E_{phobic}(\phi) := \int_\Omega \Big(\frac{1}{2}|\nabla\phi|^2 + \frac{1}{\varepsilon^2}F(\phi)\Big)dx$$

where E_{philic} and E_{phobic} represent the philic and phobic energies, respectively. The original model of Cahn and Hilliard [13] describe the phase separation and coarsening phenomena in a melted alloy that is quenched to a temperature at which only two different concentration phases can exist stably. In this case, the phobic (or chemical) free energy density was given by (1.3).

To derive the Cahn-Hilliard equation, the starting point is the mass balance law

$$\phi_t + \gamma\,\nabla\cdot J = 0,$$

where $\gamma > 0$ denotes a relaxation time constant, J is the phase flux defined as

$$J = -M(\phi)\nabla\left(\frac{\partial E(\phi)}{\partial \phi}\right),$$

and $M(\phi)$ represents the so-called mobility function. For more physical background, derivation and discussion of the Cahn-Hilliard equation we refer to [9, 60].

From now on, we are going to consider a constant value for the mobility $M(\phi) = 1$ and the Ginzburg-Landau double well potential for the phobic free energy,

$$F(\phi) = \frac{1}{4}(\phi^2 - 1)^2, \tag{2.4}$$

with

$$f(\phi) = F'(\phi) = (\phi^2 - 1)\phi.$$

Under these assumptions, the Cahn-Hilliard problem reads,

$$\begin{cases} \phi_t = \gamma\Delta(-\Delta\phi + \frac{1}{\varepsilon^2}f(\phi)) & \text{in } \Omega \times (0,T), \\ \dfrac{\partial\phi}{\partial n} = 0, \quad \dfrac{\partial(-\Delta\phi + \frac{1}{\varepsilon^2}f(\phi))}{\partial n} = 0 & \text{on } \partial\Omega \times (0,T), \\ \phi|_{t=0} = \phi_0 & \text{in } \Omega. \end{cases}$$

In order to avoid the problems related to the fourth order derivative,we rewrite the problem using the chemical potential as an auxiliary unknown (see for instance [20, 27])

$$(P) \qquad \begin{cases} \phi_t = \gamma\Delta w, \qquad w = -\Delta\phi + \dfrac{1}{\varepsilon^2}f(\phi), & \text{in } \Omega \times (0,T), \\ \dfrac{\partial\phi}{\partial n} = 0, \quad \dfrac{\partial w}{\partial n} = 0, & \text{on } \partial\Omega \times (0,T), \\ \phi|_{t=0} = \phi_0, & \text{in } \Omega. \end{cases}$$

The weak formulation of problem (P) is defined as follows: Find (ϕ, w) such that

$$\phi \in L^\infty(0,T;H^1(\Omega)), \quad \phi_t \in L^2(0,T;(H^1(\Omega))') \quad \text{and} \quad w \in L^2(0,T;H^1(\Omega))$$

and satisfying the following variational formulation

$$(VP) \qquad \begin{cases} \langle \phi_t, \bar{w}\rangle + \gamma(\nabla w, \nabla \bar{w}) = 0 & \forall\, \bar{w} \in H^1(\Omega), \\ (w, \bar{\phi}) = (\nabla\phi, \nabla\bar{\phi}) + \dfrac{1}{\varepsilon^2}(f(\phi), \bar{\phi}) & \forall\, \bar{\phi} \in H^1(\Omega). \end{cases}$$

Hereafter, the scalar product in the $L^2(\Omega)$-space will be denoted by $(f,g) := \int_\Omega f(x)g(x)dx$ and the duality product between $(H^1(\Omega))'$ and $H^1(\Omega)$ will be denoted by $\langle \phi_t, \bar{w}\rangle$.

The total mass is conserved in time, i.e., $\int_\Omega \phi(t)$ remains constant in time, as we can realize testing by $\bar{w} = 1$ in (VP),

$$\frac{d}{dt}\int_\Omega \phi = 0, \qquad i.e. \quad \int_\Omega \phi(t) = \int_\Omega \phi_0 \quad \forall\, t \geq 0. \tag{2.5}$$

Moreover, taking $\bar{w} = w$ and $\bar{\phi} = \phi_t$ in (VP), we arrive at the energy law

$$\frac{d}{dt}E(\phi(t)) + \gamma \int_\Omega |\nabla w(t)|^2 dx = 0. \tag{2.6}$$

Expression (2.6) implies that the energy decreases in time with a rate given by the physical dissipation $\gamma\|\nabla w(t)\|^2_{L^2}$. From these properties is possible to deduce the existence and uniqueness of global in time weak solution (ϕ, w) of (P), [1, 8, 28, 31, 46] and it is known that this system does not satisfy a maximum principle property: " $|\phi(t,x)| < 1$ *a.e. in* Ω *for each* $t \geq 0$ *if the initial data satisfies* $|\phi_0(x)| < 1$ *a.e. in* Ω ". On the other hand, there are two particular cases where the Cahn-Hilliard problem satisfy a maximum principle :

1. Considering the polynomial potential (1.2) and a degenerated mobility (vanishing when the phase takes the values ± 1). This case is studied in [27] where the authors present a result for the existence of solution.

2. Considering the logarithmic potential (1.3). In this case, the maximum principle property $\phi(t) \in (-1, 1)$ holds, given by the singularity of the potential at $\phi = \pm 1$, because $F'(\pm 1) = +\infty$ introduces a "barrier" at $\phi = \pm 1$.

2.1 A generic second order scheme

In this section, we present a generic second order in time approximation of system (VP), that will be used to present different schemes introduced in the literature. Assume a fixed partition of the time interval $[0, T]$ given by $t^n = k\,n$ where $k > 0$ denotes the time step (that we take constant for simplicity). Let consider $\phi^0 = \phi_0 = \phi(t^0)$ (and in the case of a two-step scheme we compute ϕ^1 by means of an one-step scheme). Then, the scheme reads: Given $(\phi^{n-1}, \phi^n) \in H^1(\Omega)^2$, find $(\phi^{n+1}, w^{n+\frac{1}{2}}) \in H^1(\Omega)^2$ such that

$$\begin{cases} \left(\delta_t \phi^{n+1}, \bar{w}\right) + \gamma(\nabla w^{n+\frac{1}{2}}, \nabla \bar{w}) = 0 \qquad \forall\, \bar{w} \in H^1(\Omega), \\ (w^{n+\frac{1}{2}}, \bar{\phi}) = (\nabla \phi^{n+\frac{1}{2}}, \nabla \bar{\phi}) + \dfrac{1}{\varepsilon^2}(f^k(\phi^{n+1}, \phi^n), \bar{\phi}) \qquad \forall\, \bar{\phi} \in H^1(\Omega). \end{cases} \tag{2.7}$$

Hereafter $\delta_t \phi^{n+1} := (\phi^{n+1} - \phi^n)/k$. The unknown $w^{n+\frac{1}{2}}$ is an approximation at midpoint $t^{n+\frac{1}{2}} := (t^n + t^{n+1})/2$ (directly computed), while $\phi^{n+\frac{1}{2}} := (\phi^{n+1} + \phi^n)/2$ is a Crank-Nicolson approximation.

Taking $\bar{w} = 1$, it is possible to show that these schemes are conservative because the total mass is constant in time,

$$\int_\Omega \phi^{n+1} = \int_\Omega \phi^n = \cdots = \int_\Omega \phi^0.$$

In order to assure that previous schemes have second order in time accuracy, $f^k(\phi(t^{n+1}), \phi(t^n))$ must be a second order approximation of $f(\phi(t^{n+\frac{1}{2}}))$.

On the other hand, testing in (2.7) by $(\bar{\phi}, \bar{w}) = (\delta_t \phi^{n+1}, w^{n+\frac{1}{2}})$ we obtain the following discrete energy law (a discrete version of (2.6)):

$$\delta_t E(\phi^{n+1}) + \gamma \|\nabla w^{n+\frac{1}{2}}\|_{L^2}^2 + \frac{1}{\varepsilon^2} ND_{phobic}^{n+1} = 0, \tag{2.8}$$

where

$$\delta_t E(\phi^{n+1}) = \frac{E(\phi^{n+1}) - E(\phi^n)}{k}$$

and

$$ND_{phobic}^{n+1} = \frac{1}{k} \int_\Omega f^k(\phi^{n+1}, \phi^n)(\phi^{n+1} - \phi^n) - \frac{1}{k} \int_\Omega (F(\phi^{n+1}) - F(\phi^n)). \tag{2.9}$$

In particular, depending on the approximation considered of $f^k(\phi^{n+1}, \phi^n)$ we will obtain different numerical schemes, with different discrete energy laws.

Definition 2.1 *The numerical scheme* (2.7) *is energy-stable if the following relation holds*

$$\delta_t E(\phi^{n+1}) + \gamma \|\nabla w^{n+\frac{1}{2}}\|_{L^2}^2 \leq 0, \quad \forall\, n.$$

Definition 2.2 *The numerical scheme* (2.7) *is energy-decreasing if the following relation holds*

$$E(\phi^{n+1}) \leq E(\phi^n), \quad \forall\, n.$$

Remark 2.3 *In particular, each energy-stable scheme is also energy-decreasing, but the contrary is not true in general. The more restrictive energy-stability criterion let us isolate the influence of physical dissipation $\gamma \|\nabla w\|_{L^2}^2$ from the numerical perturbations.*

3 Numerical Methods for the Cahn-Hilliard equation

In this section, we review different numerical approximations that have been introduced in the literature during the last years. We are going to organize this section in three main parts: The first part is devoted to present the nonlinear approximations of the potential term $f^k(\phi^{n+1}, \phi^n)$, while the second part focuses on linear approximations of this term. Finally, in the third part of the section we will introduce adaptive time step algorithms that have been proposed in the literature.

3.1 Nonlinear Schemes

Nonlinear schemes have been widely used to approximate the potential term $f^k(\phi^{n+1}, \phi^n)$ due to the good properties that they can show with respect the energy stability of the schemes. However, it is important to point out that there are several drawbacks when you consider these approximations. The first one is with regards the computational cost of the simulations, because an iterative method is needed to approximate the schemes, increasing the number of

iterations during the simulations (if you compare with linear schemes). Another issue that is important (and sometimes is not well stablished in the literature) is the fact that when you use an iterative method to approximate the nonlinear scheme, some constraints may appear to assure the existence of solution and the convergence of the *iterated* solution to the *nonlinear* one.

3.1.1 Eyre approximation (E1)

The key point in Eyre's work [29] is to approximate the potential term introducing positive phobic numerical dissipation in the discrete energy law (2.8) to assure the unconditional energy-stability of the scheme. For this purpose he splits the potential term in a convex and a non-convex part

$$F(\phi) = F_c(\phi) + F_e(\phi) \quad \text{with} \quad F_c''(\phi) \geq 0 \quad \text{and} \quad F_e''(\phi) \leq 0 \quad \forall\, \phi \in \mathbb{R}. \tag{3.10}$$

Indeed, when we consider the potential (2.4) it is possible to take $F_c(\phi) = (\phi^4 + 1)/4$ and $F_e(\phi) = -\phi^2/2$. Then, the (nonlinear) Eyre's method is a first order scheme, implicit for the diffusion part

$$\begin{cases} \left(\delta_t \phi^{n+1}, \bar{w}\right) + \gamma(\nabla w^{n+1}, \nabla \bar{w}) = 0 \qquad \forall\, \bar{w} \in H^1(\Omega), \\ (w^{n+1}, \bar{\phi}) = (\nabla \phi^{n+1}, \nabla \bar{\phi}) + \dfrac{1}{\varepsilon^2}(f^k(\phi^{n+1}, \phi^n), \bar{\phi}) \qquad \forall\, \bar{\phi} \in H^1(\Omega). \end{cases} \tag{3.11}$$

taking implicitly the convex term (or contractive) and implicitly the non-convex one (or expansive), i.e.

$$f^k(\phi^{n+1}, \phi^n) = F_c'(\phi^{n+1}) + F_e'(\phi^n). \tag{3.12}$$

In particular, in our case the approximation reads

$$f^k(\phi^{n+1}, \phi^n) = (\phi^{n+1})^3 - \phi^n.$$

Theorem 3.1 *Scheme* (3.11) *with the potential approximation* (3.12) *is unconditionally energy-stable and first order accurate in time.*

3.1.2 Midpoint approximation (MP)

The modified midpoint approximation of the potential term

$$f^k(\phi^{n+1}, \phi^n) = \frac{F(\phi^{n+1}) - F(\phi^n)}{\phi^{n+1} - \phi^n} \tag{3.13}$$

has been widely used in the literature [26, 20, 56] to design one-step unconditionally energy-stable schemes preserving the discrete energy law, i.e., without introducing phobic numerical

dissipation in the energy law ($ND^{n+1}_{phobic} = 0$). In particular, in the case of polynomial potential (2.4) it is possible to factorize (3.13), arriving at

$$f^k(\phi^{n+1}, \phi^n) = \frac{1}{4}[(\phi^{n+1} + \phi^n)((\phi^{n+1})^2 + (\phi^n)^2)] - \frac{1}{2}(\phi^{n+1} + \phi^n).$$

Theorem 3.2 *Scheme* (2.7) *with the potential approximation* (3.13) *is unconditionally energy-stable. In particular, the following discrete energy laws hold:*

$$\delta_t E(\phi^{n+1}) + \gamma \|\nabla w^{n+1/2}\|^2_{L^2} = 0. \tag{3.14}$$

Theorem 3.3 (Conditional unique solvability) *Under the constraint*

$$k < 4\varepsilon^4/\gamma$$

there exists an unique solution of scheme (2.7) *with the potential approximation* (3.13).

In order to approximate the nonlinear scheme (2.7)-(3.13) it is necessary to implement an iterative algorithm. In [38] the authors have studied the case of approximating the nonlinear scheme using Newton's algorithm. For this purpose, we can consider a Galerkin approximation of the problem (for instance with a Finite Element approximation is space):
Given $(\psi^l, z^l) \in X_h \times W_h$ (assuming $(\psi^0, z^0) = (0, z^{n-\frac{1}{2}})$ at the first step), to calculate $(\psi^{l+1}, z^{l+1}) \in X_h \times W_h$ solving

$$\begin{cases} (\psi^{l+1}, \bar{z}) + \gamma\, k\Big(\nabla z^{l+1}, \nabla \bar{z}\Big) = 0, \\ \frac{1}{2}(\nabla\psi^{l+1}, \nabla\bar{\psi}) + \frac{1}{\varepsilon^2}\left(\frac{\partial f^k}{\partial \phi^{n+1}}(\psi^l + \phi^n, \phi^n)\psi^{l+1} - \oint_\Omega \frac{\partial f^k}{\partial \phi^{n+1}}(\psi^l + \phi^n, \phi^n)\psi^{l+1}, \bar{\psi}\right) \\ -(z^{l+1}, \bar{\psi}) = -(\nabla\phi^n, \nabla\bar{\psi}) + \frac{1}{\varepsilon^2}\left(\frac{\partial f^k}{\partial \phi^{n+1}}(\psi^l + \phi^n, \phi^n)\psi^{l} - \oint_\Omega \frac{\partial f^k}{\partial \phi^{n+1}}(\psi^l + \phi^n, \phi^n)\psi^{l}, \bar{\psi}\right) \\ -\frac{1}{\varepsilon^2}\left(f^k(\psi^l + \phi^n, \phi^n) - \oint_\Omega f^k(\psi^l + \phi^n, \phi^n), \bar{\psi}\right), \end{cases} \tag{3.15}$$

for each $(\bar{\psi}, \bar{z}) \in X_h \times W_h$, until $\|\psi^{l+1} - \psi^l\|_{H^1} \leq tol$. In [38] the following results are proved:

Theorem 3.4 (Existence of solution of Newton's method) *There exists a unique solution of the iterative algorithm* (3.15) *under the constraint* $k < 4\varepsilon^4/\gamma$.

Theorem 3.5 (Convergence of Newton's method) *The sequence of solutions* $\{(\psi^l, z^l)\}_{l\geq 0}$ *of the iterative algorithm* (3.15) *converges to the solution* $(\psi^{n+1}, z^{n+\frac{1}{2}})$ *of scheme* (2.7) *with the potential* (3.13) *in the* $H^1(\Omega)$*-norm in a quadratic way under the constraints*

$$\frac{k^{1/2}}{\varepsilon^4} < C \quad \text{and} \quad \lim_{(k,h)\to 0} \frac{k}{h^2} = 0.$$

3.1.3 Gomez-Hughes approximation (GH)

In [35], the authors presented a second-order accurate time integration algorithm for the Cahn-Hilliard equation, based in the following quadrature formulas (also introduced by them)

$$\int_a^b g(x)dx = \frac{(b-a)}{2}\Big(g(a)+g(b)\Big) - \frac{(b-a)^3}{12}g''(a) - \frac{(b-a)^4}{24}g'''(\xi), \quad \xi \in (a,b). \tag{3.16}$$

and

$$\int_a^b g(x)dx = \frac{(b-a)}{2}\Big(g(a)+g(b)\Big) - \frac{(b-a)^3}{12}g''(b) + \frac{(b-a)^4}{24}g'''(\eta), \quad \eta \in (a,b). \tag{3.17}$$

They presented this approximation using the *logarithmic potential* (1.3), although this formulation can be considered with any kind of potentials, including the case of the *polynomial potential* (2.4) that we are considering in this work. The main idea is to split the potential following the convexity of their second derivatives, i.e., if we consider a generic potential $F(\phi)$, we can always take (although this splitting may not be unique):

$$F(\phi) = F_1(\phi) + F_2(\phi)$$

such that

$$F_1^{iv}(\phi) \geq 0 \quad \text{and} \quad F_2^{iv}(\phi) \leq 0.$$

Then the approximation proposed is (where $f_i(\phi) = F_i'(\phi)$, $i = 1, 2$)

$$f^k(\phi^{n+1}, \phi^n) = \frac{1}{2}\Big(f(\phi^n) + f(\phi^{n+1})\Big) - \frac{(\phi^{n+1}-\phi^n)^2}{12}\Big(f_1''(\phi^n) + f_2''(\phi^{n+1})\Big). \tag{3.18}$$

In particular, in the quartic polynomial case, if we consider

$$F_1(\phi) = \frac{1}{4}(\phi^4+1), \quad F_2(\phi) = -\frac{1}{2}\phi^2 \qquad \Big(F_1^{iv}(\phi) = 6 \geq 0, \quad F_2^{iv}(\phi) = 0 \leq 0\Big),$$

then the approximation reads

$$f^k(\phi^{n+1}, \phi^n) = \frac{1}{2}\left[(\phi^{n+1})^3 - (\phi^n)^2\phi^n + 2\phi^{n+1}(\phi^n)^2\right] - \frac{1}{2}(\phi^{n+1}+\phi^n).$$

Theorem 3.6 *Scheme* (2.7) *with the potential approximation* (3.18) *is unconditionally energy-stable. In fact, in this case:*

$$ND_{phobic}^{n+1} = \frac{1}{k}\frac{1}{4}\int_\Omega (\phi^{n+1}-\phi^n)^4 dx = \frac{k^3}{4}\int_\Omega (\delta_t\phi^{n+1})^4 dx$$

Furthermore, the scheme gives rise to a local truncation error

$$\tau(t^{n+1}) = f(\phi(t^{n+\frac{1}{2}})) - f^k(\phi(t^{n+1}), \phi(t_n))$$

with second order accuracy, i.e. $|\tau(t^{n+1})| \leq C\,k^2$, *with* C *independent of* k *and* n.

Remark 3.7 *Potential approximation* (3.18) *has second order accuracy towards* $f(\phi(t^{n+\frac{1}{2}}))$, *but provides a third order numerical dissipation with respect to the energy-stability.*

3.1.4 Taylor expansion of the midpoint approach (TE)

Another approach considered in the literature that introduces some positive numerical dissipation has been considered in [49] for a Navier-Stokes-Cahn-Hilliard problem, where the key point is to consider the Taylor expansion of the potential term (3.13). The potential approximation proposed is:

$$f^k(\phi^{n+1},\phi^n) = f(\phi^{n+1}) - \frac{1}{2}f'(\phi^{n+1})(\phi^{n+1}-\phi^n) + \frac{1}{3!}f''(\phi^{n+1})(\phi^{n+1}-\phi^n)^2. \tag{3.19}$$

In particular, in our case the approximation reads

$$f^k(\phi^{n+1},\phi^n) = \frac{1}{2}[(\phi^{n+1})^3 - (\phi^{n+1})^2\phi^n + 2\phi^{n+1}(\phi^n)^2] - \frac{1}{2}(\phi^{n+1}+\phi^n).$$

Theorem 3.8 *Scheme* (2.7) *with the potential approximation* (3.19) *is unconditionally energy-stable. In fact, in this case:*

$$ND^{n+1}_{phobic} = \frac{1}{k}\frac{1}{4}\int_\Omega (\phi^{n+1}-\phi^n)^4 dx = \frac{k^3}{4}\int_\Omega (\delta_t\phi^{n+1})^4 dx$$

Furthermore, the scheme gives rise to a local truncation error with second order accuracy.

Remark 3.9 *Potential approximation* (3.19) *has second order accuracy towards* $f(\phi(t^{n+\frac{1}{2}}))$*, but provides a third order numerical dissipation with respect to the energy-stability.*

3.1.5 (MP-BDF2)

In [61], the authors derive a second order approximation of the potential term to define unconditionally energy-stable schemes for a thin film epitaxy model. The basic idea is take into account that the energy density $F(\phi)$ is smooth and possesses a convex(+) plus a concave (−) decomposition as

$$F(\phi) = F_+(\phi) + F_-(\phi)$$

such that

$$F_+(\phi) = \frac{1}{4}(\phi^4+1), \qquad F_-(\phi) = -\frac{1}{2}\phi^2.$$

The philosophy to construct a second-order energy-stable scheme is to approximate the convex and the non-convex terms using different second order approximations. In particular, treating the convex part using the midpoint approximation **(MP)** (presented in (3.13)) and the non-convex part using a Backward Difference Formula **(BDF2)** (which is an explicit second order two-step approximation at $t^{n+\frac{1}{2}}$),

$$f^k_-(\phi^n,\phi^{n-1}) = \frac{3}{2}F'_-(\phi^n) - \frac{1}{2}F'_-(\phi^{n-1}) = -\frac{1}{2}\left(3\phi^n - \phi^{n-1}\right)$$

Therefore,

$$\begin{aligned} f^k(\phi^{n+1},\phi^n,\phi^{n-1}) &= f_+^k(\phi^{n+1},\phi^n)+f_-^k(\phi^n,\phi^{n-1}) \\ &= \frac{1}{4}\Big[(\phi^{n+1})^3+(\phi^{n+1})^2\phi^n+(\phi^n)^2\phi^{n+1}+(\phi^n)^3\Big]-\frac{1}{2}\Big(3\phi^n-\phi^{n-1}\Big) \end{aligned} \tag{3.20}$$

It is easy to check that approximation (3.20) has second order accuracy towards $f(\phi(t^{n+\frac{1}{2}}))$.

Theorem 3.10 *Using the potential approximation* (3.20)*, scheme* (2.7) *is unconditionally energy-stable for a modified energy* $\widetilde{E}(\phi^{n+1})$*. In fact, the following discrete energy law holds:*

$$\delta_t\widetilde{E}(\phi^{n+1})+\frac{1}{\varepsilon^2}\widetilde{ND}_{phobic}^{n+1}+\gamma\|\nabla w^{n+1/2}\|_{L^2}^2=0 \tag{3.21}$$

for the modified energy

$$\widetilde{E}(\phi^{n+1})=\int_\Omega\left(\frac{1}{2}|\nabla\phi^{n+1}|^2+\frac{1}{\varepsilon^2}F(\phi^{n+1})+\frac{k^2}{4\varepsilon^2}|\delta_t\phi^{n+1}|^2\right)dx$$

and

$$\widetilde{ND}_{phobic}^{n+1}=\frac{k^3}{4}\|\delta_{tt}\phi^{n+1}\|_{L^2}^2.$$

where $\delta_{tt}\phi^{n+1}=\delta_t(\delta_t\phi^{n+1})=(\delta_t\phi^{n+1}-\delta_t\phi^n)/k$.

Remark 3.11 *Notice that* $\widetilde{E}(\phi^{n+1})=E(\phi^{n+1})+E_{pert}(\phi^{n+1})$ *where*

$$E_{pert}(\phi^{n+1})=\frac{k^2}{4\varepsilon^2}\|\delta_t\phi^{n+1}\|_{L^2}^2$$

is a perturbation of the "exact" energy $E(\phi^{n+1})$*.*

Since the non-convex part is treated explicitly, one has the following result:

Theorem 3.12 (Unconditional unique solvability) *Scheme* (2.7) *with the potential approximation given in* (3.20) *is uniquely solvable.*

In order to approximate the nonlinear scheme (2.7)-(3.20) it is necessary to implement an iterative algorithm. In [38] the case of approximating the nonlinear scheme using Newton's algorithm have been studied. For this purpose, we can consider a Galerkin approximation of the problem (for instance with a Finite Element approximation):
Given $(\psi^l,z^l)\in X_h\times W_h$ (assuming $(\psi^0,z^0)=(0,z^{n-\frac{1}{2}})$ at the first step), to calculate $(\psi^{l+1},z^{l+1})\in$

$X_h \times W_h$ solving

$$\begin{cases} (\psi^{l+1}, \bar{z}) + k\,\gamma\Big(\nabla z^{l+1}, \nabla \bar{z}\Big) = 0, \\ \frac{1}{2}(\nabla\psi^{l+1}, \nabla\bar{\psi}) + \left(\frac{\partial f_+^k}{\partial \phi^{n+1}}(\psi^l + \phi^n, \phi^n)\cdot\psi^{l+1} - \oint_\Omega \frac{\partial f_+^k}{\partial \phi^{n+1}}(\psi^l + \phi^n, \phi^n)\cdot\psi^{l+1}, \bar{\psi}\right) \\ -(z^{l+1}, \bar{\psi}) = -(\nabla\phi^n, \nabla\bar{\phi}) - \left(f_-^k(\phi^n, \phi^{n-1}) - \oint_\Omega f_-^k(\phi^n, \phi^{n-1}), \bar{\psi}\right) \\ + \left(\frac{\partial f_+^k}{\partial \phi^{n+1}}(\psi^l + \phi^n, \phi^n)\cdot\phi^l - \oint_\Omega \frac{\partial f_+^k}{\partial \phi^{n+1}}(\psi^l + \phi^n, \phi^n)\cdot\phi^l, \bar{\psi}\right) \\ - \left(f_+^k(\psi^l + \phi^n, \phi^n) - \oint_\Omega f_+^k(\psi^l + \phi^n, \phi^n), \bar{\psi}\right), \end{cases} \tag{3.22}$$

for each $(\bar{\psi}, \bar{z}) \in X_h \times W_h$ until $\|\psi^{l+1} - \psi^l\|_{H^1} \leq tol$. In [38] the following results are proved:

Theorem 3.13 (Existence of solution of Newton's method) *There exists an unique solution of the iterative algorithm* (3.22).

Theorem 3.14 (Convergence of Newton's method) *The sequence of solutions* $\{(\psi^l, z^l)\}_{l\geq 0}$ *of the iterative algorithm* (3.22) *converges to the solution* $(\psi^{n+1}, z^{n+\frac{1}{2}})$ *of scheme* (2.7)-(3.20) *in* $H^1(\Omega)$*-norm under the constraints*

$$\frac{k^{1/2}}{\varepsilon^4} < C \quad \text{and} \quad \lim_{(k,h)\to 0} \frac{k}{h^2} = 0.$$

3.2 Linear Schemes

In order to be able to obtain meaningful simulations in the phase field framework, we usually need to compute large amount of time steps, and by extension this fact usually implies a high computational cost. And if you also need to approximate a nonlinear scheme for each iteration then the simulation could become a very tedious work. With this in mind, researchers have started to think in efficient ways of designing linear schemes to reduce this computational work. But we should keep in mind that these schemes are *linearizing* a nonlinear equation and some limitations in terms of accuracy or approximation should arise. In the following, we outline the linear approximations of the potential term $f^k(\phi^{n+1}, \phi^n)$ that have been presented in the literature pointing out the limitations of each of the related schemes.

3.2.1 Linear Eyre approximation (EL1)

In order to obtain linear schemes following the ideas of Eyre [29], the authors in [37] rewrite the potential part of the free energy using a parameter $\beta \geq 0$, as follows:

$$F(\phi) = \frac{1}{4}(\phi^2 - 1)^2 = \frac{1}{4}(\phi^4 + 2\beta\phi^2 - 2(\beta+1)\phi^2 + 1),$$

Then, they consider the following separation of the potential,

$$F_1(\phi) = \frac{1}{2}\beta\phi^2 \qquad \text{and} \qquad F_2(\phi) = \frac{1}{4}(\phi^4 - 2(\beta+1)\phi^2 + 1).$$

Thus, the potential approximation of the potential reads

$$f^k(\phi^{n+1}, \phi^n) = F_1'(\phi^{n+1}) + F_2'(\phi^n). \tag{3.23}$$

Indeed, the scheme considering $\beta = 2$ was introduced in [29].

Theorem 3.15 *Using the potential approximation* (3.23)*, scheme* (2.7) *satisfies*

$$ND_{phobic}^{n+1} \geq 0 \Longleftrightarrow |\phi|^2 \leq (2\beta+1)/3.$$

Remark 3.16 *It is not clear that we can assure $ND_{phobic}^{n+1} \geq 0$ due the non-existence of a maximum principle for the Cahn-Hilliard model.*

Remark 3.17 *The natural idea to assure the energy-stability of the scheme is consider β large enough that will imply $ND_{phobic}^{n+1} \geq 0$ almost for sure. But in [37] it is shown how the introduction of too much numerical dissipation usually leads to wrong equilibrium solutions.*

Remark 3.18 *In the last years, the introduction of an extra dissipative term $\frac{S}{\varepsilon^2}(\phi^{n+1} - \phi^n)$ to Euler's schemes and the idea of considering a truncated potential $\widetilde{F}$ such that the second derivative of this truncated potential is bounded ($|\widetilde{F}''(\phi)| \leq M$ for each $\phi \in \mathbb{R}$) have been widely used (see for instance [63]), obtaining energy-stable schemes for a choice of S depending on M. It is interesting to note that this kind of schemes could be seen as Eyre's linear schemes.*

3.2.2 Optimal Dissipation approximation (OD2)

In [37], the authors develop the so-called optimal dissipation approach, a second order in time linear approximation of the potential term derived by using the following Hermite quadrature formula (exact for $\mathbb{P}_1$),

$$\int_a^b g(x)dx = (b-a)g(a) + \frac{1}{2}(b-a)^2 g'(a) \; + \; C\,(b-a)^3 g''(\xi). \tag{3.24}$$

In fact, the approximation reads

$$f^k(\phi^{n+1}, \phi^n) = f(\phi^n) + \frac{1}{2}f'(\phi^n)(\phi^{n+1} - \phi^n) = \frac{3}{2}(\phi^n)^2\phi^{n+1} - \frac{1}{2}(\phi^n)^3 - \frac{\phi^{n+1} + \phi^n}{2}. \tag{3.25}$$

Using this approximation in (2.7) we get a second order linear scheme where the numerical dissipation introduced in the discrete energy law has also second order accuracy in each time step. It is optimal from the phobic numerical dissipation point of view due the impossibility of designing a linear approximation introducing a higher order in time phobic numerical dissipation. The problem is that is not possible to control the sign of ND_{phobic}^{n+1} to derive the unconditional stability of the scheme.

Theorem 3.19 (Conditional unique solvability) *Scheme* (2.7) *with the potential approximation given in* (3.25)*, is unique solvable under the constraint*

$$k < 2\varepsilon^4/\gamma.$$

3.2.3 (OD2-BDF2)

It is possible to develop an approach for the potential term combining some of the ideas used to derive the **(MP-BDF2)** and **(OD2)** approximations [38]. The first idea consists in splitting again the potential term between convex and non-convex part, then the convex part is approximated using **(OD2)**, while a two-steps backward differences formula **(BDF2)** is considered for the non-convex part as in (3.20), i.e.,

$$f^k(\phi^{n+1},\phi^n,\phi^{n-1}) = f_+^k(\phi^{n+1},\phi^n) + f_-^k(\phi^n,\phi^{n-1})$$

where

$$\begin{array}{rcccl} f_+^k(\phi^{n+1},\phi^n) & = & f_+^k(\phi^n) + \dfrac{1}{2} f_+^k(\phi^n)(\phi^{n+1}-\phi^n) & = & \dfrac{1}{2}\left[3(\phi^n)^2\phi^{n+1} - (\phi^n)^3\right], \\ f_-^k(\phi^n,\phi^{n-1}) & = & \dfrac{3}{2} f_-^k(\phi^n) - \dfrac{1}{2} f_-^k(\phi^{n-1}) & = & -\dfrac{1}{2}\left(3\phi^n - \phi^{n-1}\right). \end{array} \tag{3.26}$$

This approximation has a truncature error of second order in time and the numerical dissipation introduced in the discrete energy law is also second order in each time step

$$ND_{phobic}^{n+1} = O(k^2),$$

but it is not possible to control the sign of ND_{phobic}^{n+1} (as in the **(OD2)** case). Again, the open problem about the energy-stability could be studied.

On the other hand, following the argument of Theorem 3.19, since now the non-convex part is treated explicitly, we have the following result:

Theorem 3.20 (Unconditional unique solvability) *Scheme* (2.7) *with the potential approximation given in* (3.26) *is uniquely solvable.*

3.2.4 Wu-Van Zwieten-Van der Zee approximation (WVV)

In [67], the authors consider the Cahn-Hilliard equation and a diffuse-interface tumor-growth system consisting of a reactive Cahn-Hilliard equation and a reaction-diffusion equation. The schemes are of the Crank-Nicolson type with a convex-concave splitting of the free-energy, and an artificial diffusivity stabilization (they introduce the term $\alpha_1\, k(\nabla\phi^{n+1}, \nabla\bar{w})$ in $(2.7)_2$).

The potential term is approximated employing an implicit Taylor expansion of the convex part and an explicit Taylor expansion of the non-convex part. The splitting considered for the

potential term is

$$F(\phi) = F_c(\phi) - F_e(\phi) = \begin{cases} \left(\phi^2 + \frac{1}{4}\right) - \left(-2\phi - \frac{3}{4}\right) & \phi < -1, \\ \left(\phi^2 + \frac{1}{4}\right) - \left(\frac{3}{2}\phi^2 - \frac{1}{4}\phi^4\right) & \phi \in [-1, 1], \\ \left(\phi^2 + \frac{1}{4}\right) - \left(2\phi - \frac{3}{4}\right) & \phi > 1. \end{cases} \tag{3.27}$$

Considering $f_c(\phi) = F_c'(\phi)$ and $f_e(\phi) = F_e'(\phi)$, the approximation of the potential term considered in the numerical scheme reads,

$$f^k(\phi^{n+1}, \phi^n) = f_c(\phi^{n+1}) - \frac{\phi^{n+1} - \phi^n}{2} f_c'(\phi^{n+1}) - f_e(\phi^n) - \frac{\phi^{n+1} - \phi^n}{2} f_e'(\phi^n), \tag{3.28}$$

where $f_c(\phi) = 2\,\phi$ and $f_e(\phi)$ is defined by parts. Then, the resulting scheme is linear.

Theorem 3.21 *If the stabilization introduced by the term $\alpha_1\, k(\nabla\phi^{n+1}, \nabla\bar{w})$ in $(2.7)_2$ is large enough, then the numerical scheme* (2.7) *with the potential approximation given in* (3.28) *is unconditionally energy-stable.*

Remark 3.22 *From the analytical point of view, the splitting* (3.27) *of $F(\phi)$ into two different cases depending on the possibility of ϕ being in the interval $[-1, 1]$ or outside this interval is very convenient, because allows to control the phobic numerical dissipation using the extra numerical dissipation introduced in the philic term. But from the convergence point of view, it is not clear that the solution for this kind of splitted potential will converge to the solution of the original problem (VP) that considers the potential $F(\phi) = (1/4)(\phi^2 - 1)^2$ because the Cahn-Hilliard problem doesn't satisfy the maximum principle.*

Remark 3.23 *Assuming just the case where $\phi \in [-1, 1]$, the approximation of the potential reads:*

$$f^k(\phi^{n+1}, \phi^n) = \frac{3}{2}(\phi^n)^2\phi^{n+1} - \frac{1}{2}(\phi^n)^3 - \frac{\phi^{n+1} + \phi^n}{2}. \tag{3.29}$$

*This approximation of the potential term exactly correspond with the **(OD2)** approximation* (3.25) *that was previously introduced in the literature in [37].*

3.2.5 Second order Lagrange multiplier scheme (LM2)

In [6], a Lagrange multiplier is introduced to penalize the restriction of unitary director vector in the Nematic Liquid Crystals framework and this idea was extended to the Cahn-Hilliard equation in [37, 38] to derive unconditionally energy-stable (for a modified energy) linear schemes. Indeed, a one-step and first order in time scheme and two two-step and second order schemes were introduced. The basic idea consists on thinking on the double potential $F(\phi)$ as a penalization

of the constraint $|\phi|^2 = 1$. Then, we can introduce $q(x,t) \in \mathbb{R}$ that is not exactly a Lagrange multiplier but allows to enforce the *sphere condition* $|\phi| = 1$, getting a linear unconditional stable and uniquely solvable scheme. Basically, the new formulation consists in taking advantage of the Ginzburg-Landau potential, writing it as

$$\frac{1}{\varepsilon^2} f(\phi) = q\phi \qquad \text{where} \qquad q = \frac{1}{\varepsilon^2}(\phi^2 - 1)$$

and consider the time derivative in the q-equation:

$$\varepsilon^2 q_t = 2\phi\phi_t$$

jointly with the initial condition $q(0) = \dfrac{1}{\varepsilon^2}(\phi(0)^2 - 1)$. The weak formulation of this problem is defined as follows: Find (ϕ, w, q) such that

$$\phi \in L^\infty(0,T; H^1(\Omega) \cap L^\infty(\Omega)), \quad \phi_t \in L^2(0,T; (H^1(\Omega))'),$$

$$w \in L^2(0,T; H^1(\Omega)), \quad q \in L^2((0,T)\times\Omega), \quad q_t \in L^2(0,T; (H^1(\Omega) \cap L^\infty(\Omega))')$$

and satisfying the following equations

$$\begin{cases} \langle \phi_t, \bar{w}\rangle + \gamma(\nabla w, \nabla \bar{w}) = 0 \qquad \forall\, \bar{w} \in H^1(\Omega), \\ (w, \bar{\phi}) = (\nabla\phi, \nabla\bar{\phi}) + (q\phi, \bar{\phi}) \qquad \forall\, \bar{\phi} \in H^1(\Omega), \\ \dfrac{\varepsilon^2}{2}\langle q_t, \bar{q}\rangle = \langle \phi\, \phi_t, \bar{q}\rangle \qquad \forall\, \bar{q} \in H^1(\Omega) \cap L^2(\Omega). \end{cases}$$

To illustrate this approach, in this work we shall focus just on one of the second order schemes, where the potential term is approximated using the solutions obtained in the two previous time steps (ϕ^n, ϕ^{n-1}), maintaining the second order accuracy in time and the linearity of the scheme.

Initialization: $(\phi^0, r^0) \in H^1(\Omega) \times L^2(\Omega)$ approximations of $(\phi(0), r(0) = ((\phi(0))^2 - 1)/\varepsilon^2)$

Step $n+1$ **(**$n \geq 1$**):** Given $(\phi^{n-1}, \phi^n, r^n)$, find $(\phi^{n+1}, w^{n+\frac{1}{2}}, r^{n+1}) \in H^1(\Omega) \times H^1(\Omega) \times L^2(\Omega)$ such that

$$\begin{cases} \left(\delta_t\phi^{n+1}, \bar{w}\right) + \gamma\left(\nabla w^{n+\frac{1}{2}}, \nabla\bar{w}\right) = 0, \\ \left(\nabla\phi^{n+\frac{1}{2}}, \nabla\bar{\phi}\right) + \left(r^{n+\frac{1}{2}}\widetilde{\phi}, \bar{\phi}\right) - \left(w^{n+\frac{1}{2}}, \bar{\phi}\right) = 0, \\ \dfrac{\varepsilon^2}{2}\left(\delta_t r^{n+1}, \bar{r}\right) - \left(\widetilde{\phi}\,\delta_t\phi^{n+1}, \bar{r}\right) = 0, \end{cases} \tag{3.30}$$

for each $(\bar{\phi}, \bar{w}, \bar{r}) \in H^1(\Omega) \times H^1(\Omega) \times L^2(\Omega)$.

The unknowns $w^{n+\frac{1}{2}}$ is a direct approximation at midpoint $t^{n+\frac{1}{2}} := (t^n + t^{n+1})/2$, while $\phi^{n+\frac{1}{2}} := (\phi^{n+1} + \phi^n)/2$ and $r^{n+\frac{1}{2}} := (r^{n+1} + r^n)/2$. Finally $\widetilde{\phi} = (3\phi^n - \phi^{n-1})/2$ (**BDF2**).

Remark 3.24 *If the choice $\widetilde{\phi} = \phi^{n+\frac{1}{2}}$ is considered, we obtain nonlinear second order schemes that are equivalent to the* ***(MP)****, because from* $(3.30)_3$ *one can arrive at the expression* $r^{n+1} = \frac{1}{\varepsilon^2}((\phi^{n+1})^2 - 1)$.

Theorem 3.25 *The scheme* (3.30) *has second order in time accuracy and it is unconditionally energy-stable for the modified energy*

$$\widetilde{E}(\phi, r) = \int_\Omega \Big(\frac{1}{2}|\nabla\phi|^2 + \frac{\varepsilon^2}{4}|r|^2\Big)dx.$$

In fact, one has

$$\delta_t \widetilde{E}(\phi^{n+1}, r^{n+1}) + \gamma\|\nabla w^{n+1/2}\|_{L^2}^2 = 0. \tag{3.31}$$

Remark 3.26 *Notice that* $\widetilde{E}(\phi, r) = E(\phi) + E_{pert}(\phi, r)$ *where*

$$E_{pert}(\phi, r) = \frac{\varepsilon^2}{4}\int_\Omega |r|^2 dx - \frac{1}{\varepsilon^2}\int_\Omega F(\phi)dx.$$

Theorem 3.27 *Scheme* (3.30) *is uniquely solvable.*

3.3 Algorithms for adapting the time step

In many phase field models, adaptive time stepping is of primordial importance due to the different time scales that arise in the dynamic of the models. The adaptive time stepping technique allows us to reduce the computational time by factors of hundreds compared to the computational time keeping the time-step size constant. This helps to enhance the efficiency while maintaining high accuracy of the solution.

In order to define an algorithm for adapting the time step, we have to take into account that in all the two-steps schemes that we have previously introduced, we need to change the way of defining $\widetilde{\phi}$ because it was designed as a linear second order approximation of ϕ with a constant time-step.

In the case of non-constant time-step, let dt^{n-1} and dt^n with $t^n = t^{n-1} + dt^{n-1}$ and $t^{n+1} = t^n + dt^n$, and we consider the following expressions:

$$\phi(t_{n-1}) = \phi(t_{n+\frac{1}{2}}) - \left(dt^{n-1} + \frac{dt^n}{2}\right)\phi_t(t_{n+\frac{1}{2}}) + O((dt^{n-1})^2 + (dt^n)^2),$$

$$\phi(t_n) = \phi(t_{n+\frac{1}{2}}) - \frac{dt^n}{2}\phi_t(t_{n+\frac{1}{2}}) + O((dt^n)^2).$$

Then

$$\left(\frac{2dt^{n-1}}{dt^n} + 1\right)\phi(t_n) - \phi(t_{n-1}) = \left(\frac{2dt^{n-1}}{dt^n}\right)\phi(t_{n+\frac{1}{2}}) + O((dt^{n-1})^2 + (dt^n)^2).$$

Therefore, we can define

$$\widetilde{\phi} = \left(\frac{dt^n}{2dt^{n-1}} + 1\right)\phi^n - \frac{dt^n}{2dt^{n-1}}\phi^{n-1}. \tag{3.32}$$

Remark 3.28 *In most of the adaptive time-step algorithm the choice of the parameters involved in the process is not a trivial task. If these parameters are not efficiently chosen, the time step could increase too much and the accuracy of the solutions could be deteriorated arriving at wrong equilibrium solutions. On the other hand, it can happen that a choice of these parameters could lead to time steps remaining too small and no improvement in the computational cost is obtained. Up to our knowledge, there are no analytical results concerning how to estimate the optimum parameters involved in time step adapting algorithms for phase field models and we claim that any advance in this direction will be really appreciated.*

3.3.1 Runge-Kutta based models

There are many works where the authors have considered algorithms related with Runge-Kutta models to develop adaptive time-steps algorithms ([7, 35, 66] and the references therein), where they also combine them with multigrid methods. In particular, we will present this approach using the algorithm presented in [35], where a NURBS-based variational formulation for the Cahn-Hilliard equation was tested on two and three dimensional problems and an adaptive time-stepping method was introduced. They show the efficiency of this algorithm presenting for the first time steady state solutions of $3D$ simulations of the spinodal decomposition. For developing their algorithm, they borrowed ideas from embedded Runge-Kutta methods. The adaptive time step strategy is:

1. Compute ϕ_{BE}^{n+1} the solution of the system using a backward Euler scheme and dt^n.
2. Compute ϕ_{α}^{n+1} using second order generalized α-method and dt^n.
3. Calculate $e^{n+1} = \|\phi_{BE}^{n+1} - \phi_{\alpha}^{n+1}\|/\|\phi_{\alpha}^{n+1}\|$
4. If $e^{n+1} > tol$ recalculate time-step size $\Delta t^n = H(e^{n+1}, dt^n)$ and goto 1)
5. else Update time-step size $\Delta t^{n+1} = H(e^{n+1}, dt^n)$ and continue

where the formula used to update the time-step size is

$$H(e, \Delta t) = \rho \left(\frac{tol}{e} \right)^{1/2} dt$$

3.3.2 Guillen-Tierra

In [38], we propose an adaptive-in-time method where the time step is selected by using an criterion related to the "residual dissipation" of the discrete energy laws. We show the efficiency of this algorithm for different numerical schemes and comparing with the case of constant time

step the number of linear systems needed to be solved in order to reach the equilibrium solution. They define the residuals of the energies equalities at $t^{n+1/2}$ as:

$$RE^{n+1} = \frac{E(\phi^{n+1}) - E(\phi^n)}{dt^n} + \gamma \int_\Omega |\nabla w^{n+1/2}|^2 dx$$

Then, the time-adapting algorithm in the $(n+1)$ time-step, with $n \geq 1$, reads:
Given ϕ^n, ϕ^{n-1},dt^{n-1}, dt^n and a parameter $\theta > 1$:

1. Compute ϕ^{n+1} with $\widetilde{\phi}$ given by (3.32) and compute RE^{n+1}.
2. If $|RE^{n+1}| >$ **resmax**, take $dt^n = dt^n/\theta$ and go to 1).
3. If $|RE^{n+1}| <$ **resmin**, take $dt^{n+1} = \theta dt^n$.
4. Take $t^{n+1} = t^n + dt^n$ and go to next time step.

4 Extension of the numerical methods to vectorial potentials.

The aim of this section is to show that the ideas presented for the Cahn-Hilliard equation can be extended to other type of systems that model other kind of physical phenomena.

Although it seems that these days the communication between researchers is rapidly increasing, it can be observed in the literature that sometimes researchers from different communities have been working on parallel arriving to the same ideas without being aware that these ideas have been already presented in a different framework.

In order to illustrate this fact, we will focus on the case of the Nematic Liquid Crystals. These systems have attracted the attention of a big community of researchers for decades and in the last years it can be said that the interest in this topic has even grow.

This section is organized as follows. First, we will give a brief physical introduction to these systems and we summarize the main analytical results that can be found in the literature. Then, we present a generic second order scheme that will be used to list the different numerical schemes that have been previously introduced in the literature and their relation with the schemes presented for the Cahn-Hilliard. Finally, we will comment how to extend the rest of schemes presented for the Cahn-Hilliard equation to the Nematic Liquid Crystals framework. Indeed, we present the ideas in the Nematic case (i.e. $\boldsymbol{f}_\varepsilon^k(\boldsymbol{d}^{n+1}, \boldsymbol{d}^n)$) but their extension to other vectorial potentials that appear in the literature should be rather standard.

4.1 Nematic Liquid Crystals

Liquid Crystals are a state of matter that have properties between liquids and solids. They can behave like liquids (macroscopically), but their molecules have an orientational property (microscopically), due to elasticity effects (in particular, LCs are anisotropic liquids).

Liquid Crystals can be thermotropic and lyotropic, which change of state varying the temperature or the concentration, respectively.

Nematic phases are composed by rod-shaped molecules that have no positional order, but they self-align to have long-range directional order with their long axes roughly parallel. Thus, the molecules are free to flow and their center of mass positions are randomly distributed as in a liquid, but still maintain their long-range directional order. Most Nematics are uniaxial: they have one axis that is longer and preferred.

For uni-axial orientated Nematic Liquid Crystals, this order variable reduces to a unitary vector $\boldsymbol{d}$ representing a preferential average direction of the molecules, that is $|\boldsymbol{d}| = 1$ (where $|\cdot|$ denotes the euclidean norm).

Assume Nematic Liquid Crystals filling a domain $\Omega \subset \mathbb{R}^3$ in a time interval $(0, +\infty)$. We denote $Q = (0, +\infty) \times \Omega$ and $\Sigma = (0, +\infty) \times \partial\Omega$.

The problem is to obtain $\boldsymbol{u} : Q \to \mathbb{R}^3$ the velocity, $p : Q \to \mathbb{R}$ the pressure and $\boldsymbol{d} : Q \to \mathbb{R}^3$ the director vector such that verifies the following system, which is a simplification of the Ericksen-Leslie model introduced by F.H.Lin in [52]:

$$(EL) \qquad \begin{cases} \partial_t \boldsymbol{u} + \boldsymbol{u} \cdot \nabla \boldsymbol{u} - \nu \Delta \boldsymbol{u} + \nabla p + \lambda \nabla \cdot ((\nabla \boldsymbol{d})^t \nabla \boldsymbol{d}) &= 0 \quad \text{in } Q, \\ \nabla \cdot \boldsymbol{u} &= 0 \quad \text{in } Q. \\ \partial_t \boldsymbol{d} + \boldsymbol{u} \cdot \nabla \boldsymbol{d} + \gamma(-\Delta \boldsymbol{d} - |\nabla \boldsymbol{d}|^2 \boldsymbol{d}) &= 0 \quad \text{in } Q. \end{cases}$$

Here, $(\nabla \boldsymbol{d})^t \nabla \boldsymbol{d}$ is an elastic (symmetric) tensor and $-\Delta \boldsymbol{d} - |\nabla \boldsymbol{d}|^2 \boldsymbol{d}$ is the critical point equation related to the minimization problem of the (simplified) elastic energy $E_{ela}(\boldsymbol{d}) := \frac{1}{2} \int_\Omega |\nabla \boldsymbol{d}|^2$ subject to the constraint $|\boldsymbol{d}| = 1$. The positive coefficients ν, λ and γ represent viscosity, elasticity and time relaxation, respectively.

This differential problem is endowed with boundary conditions on Σ: $\boldsymbol{u}(t, \boldsymbol{x}) = 0$ on Σ (non-slip) and Dirichlet, Neumann or Periodic boundary conditions for $\boldsymbol{d}$ on Σ, and the initial conditions: $\boldsymbol{u}(0, \boldsymbol{x}) = \boldsymbol{u}_0(\boldsymbol{x}), \quad \boldsymbol{d}(0, \boldsymbol{x}) = \boldsymbol{d}_0(\boldsymbol{x}), \quad \boldsymbol{x} \in \Omega$. Here $\boldsymbol{u}_0 : \Omega \to \mathbb{R}^3$ such that $\nabla \cdot \boldsymbol{u}_0 = 0$ a.e. in Ω, and $\boldsymbol{d}_0 : \Omega \to \mathbb{R}^3$ such that $|\boldsymbol{d}_0| = 1$ a.e. in Ω are given functions.

Note that, the constraints $|\boldsymbol{d}| = 1$ in Q is verified from the $\boldsymbol{d}$-system whenever the initial and boundary data for $\boldsymbol{d}$ are unitary. In fact, $q = -|\nabla \boldsymbol{d}|^2$ is a Lagrange multiplier associated to the constraint $|\boldsymbol{d}| = 1$.

On the other hand, this problem satisfies a dissipative Energy Law. Indeed, since the divergence of the elastic tensor can be decomposed as [53]:

$$\nabla \cdot ((\nabla \boldsymbol{d})^t \nabla \boldsymbol{d}) = \nabla \left(\frac{1}{2} |\nabla \boldsymbol{d}|^2 \right) - (\nabla \boldsymbol{d})^t (-\Delta \boldsymbol{d}),$$

then, making

$$\int_\Omega (EL)_1 \cdot \boldsymbol{u} + \lambda \int_\Omega (EL)_3 \cdot (-\Delta \boldsymbol{d} - |\nabla \boldsymbol{d}|^2 \boldsymbol{d}),$$

using that

$$\Big(\partial_t \boldsymbol{d} + (\boldsymbol{u}\cdot\nabla)\boldsymbol{d}\Big)\cdot|\nabla \boldsymbol{d}|^2\boldsymbol{d} = 0 \quad \text{(owing to } |\boldsymbol{d}| = 1)$$

and

$$\int_\Omega \partial_t \boldsymbol{d}\cdot(-\Delta \boldsymbol{d}) = \frac{d}{dt}\frac{1}{2}\|\nabla \boldsymbol{d}\|^2_{L^2}$$

(here the boundary term vanish due to the time-independent boundary condition for $\boldsymbol{d}$), one arrives at the following Energy law (for the Erickseen-Leslie model (EL)):

$$\frac{d}{dt}\Big(E_{kin}(\boldsymbol{u}) + \lambda\, E_{ela}(\boldsymbol{d})\Big) + \nu\|\nabla \boldsymbol{u}\|^2_{L^2(\Omega)} + \left\{\begin{array}{l} \lambda\gamma\|\Delta \boldsymbol{d} + |\nabla \boldsymbol{d}|^2\boldsymbol{d}\|^2_{L^2(\Omega)} \\ \frac{\lambda}{\gamma}\|\partial_t \boldsymbol{d} + (\boldsymbol{u}\cdot\nabla)\boldsymbol{d}\|^2_{L^2(\Omega)} \end{array}\right\} = 0,$$

where $E_{kin}(\boldsymbol{u}) = \frac{1}{2}\|\boldsymbol{u}\|^2_{L^2(\Omega)}$ in the kinetic energy and $E_{ela}(\boldsymbol{d}) = \frac{1}{2}\|\nabla \boldsymbol{d}\|^2_{L^2(\Omega)}$ is the elastic energy.

4.2 The penalty model: The Ginzburg-Landau problem

Since $|\boldsymbol{d}| = 1$ is a non-convex restriction, these models are often penalized with functions of Ginzburg-Landau type. In fact, let us to consider the Ginzburg-Landau penalized functional

$$F_\varepsilon(\boldsymbol{d}) = \frac{1}{4\varepsilon^2}(|\boldsymbol{d}|^2 - 1)^2$$

where $\varepsilon > 0$ is the penalty parameter, and the corresponding gradient functional

$$\boldsymbol{f}_\varepsilon(\boldsymbol{d}) = \nabla_{\boldsymbol{d}} F_\varepsilon(\boldsymbol{d}) = \frac{1}{\varepsilon^2}(|\boldsymbol{d}|^2 - 1)\boldsymbol{d}.$$

By using the decomposition of the elastic tensor:

$$\nabla\cdot((\nabla \boldsymbol{d})^t\nabla \boldsymbol{d}) = \nabla\left(\frac{1}{2}|\nabla \boldsymbol{d}|^2 + F_\varepsilon(\boldsymbol{d})\right) - (\nabla \boldsymbol{d})^t(-\Delta \boldsymbol{d} + \boldsymbol{f}_\varepsilon(\boldsymbol{d})),$$

the penalized (Ginzburg-Landau) system can be written as:

$$(GL) \qquad \left\{\begin{array}{rcll} \partial_t \boldsymbol{u} + \boldsymbol{u}\cdot\nabla \boldsymbol{u} - \nu\Delta \boldsymbol{u} + \nabla\widetilde{p} - \lambda(\nabla \boldsymbol{d})^t(-\Delta \boldsymbol{d} + \boldsymbol{f}_\varepsilon(\boldsymbol{d})) &=& \boldsymbol{0} & \text{in } Q, \\ \nabla\cdot \boldsymbol{u} &=& 0 & \text{in } Q, \\ \partial_t \boldsymbol{d} + (\boldsymbol{u}\cdot\nabla)\boldsymbol{d} + \gamma(-\Delta \boldsymbol{d} + \boldsymbol{f}_\varepsilon(\boldsymbol{d})) &=& \boldsymbol{0} & \text{in } Q, \end{array}\right.$$

where $\widetilde{p} = p + \dfrac{\lambda}{2}|\nabla \boldsymbol{d}|^2 + \lambda\, F_\varepsilon(\boldsymbol{d})$.

Now, by using the same argument made to obtain the energy law for the (EL) model, and using now that

$$\int_\Omega \partial_t \boldsymbol{d}\cdot\boldsymbol{f}_\varepsilon(\boldsymbol{d}) = \frac{d}{dt}\int_\Omega F_\varepsilon(\boldsymbol{d})$$

one can arrive at the following energy law (for the Ginzburg-Landau model (GL)):

$$\frac{d}{dt}E_{tot}(\boldsymbol{u},\boldsymbol{d}) + \nu\|\nabla \boldsymbol{u}\|^2_{L^2(\Omega)} + \left\{\begin{array}{l} \lambda\gamma\|-\Delta \boldsymbol{d} + \boldsymbol{f}_\varepsilon(\boldsymbol{d})\|^2_{L^2(\Omega)} \\ \frac{\lambda}{\gamma}\|\partial_t \boldsymbol{d} + (\boldsymbol{u}\cdot\nabla)\boldsymbol{d}\|^2_{L^2(\Omega)} \end{array}\right\} = 0,$$

where $E_{tot}(\boldsymbol{u},\boldsymbol{d}) = E_{kin}(\boldsymbol{u}) + \lambda\, E_{ela}(\boldsymbol{d}) + \lambda E_{pen}(\boldsymbol{d})$ and $E_{pen}(\boldsymbol{d}) = \int_\Omega F_\varepsilon(\boldsymbol{d})$ is the penalized energy.

This property of (GL) model is essential to prove the existence of global in time *weak solution* of (GL) [53] (see also [54] for a more general model):

$$\boldsymbol{u} \in L^\infty(0,+\infty;\boldsymbol{L}^2(\Omega)) \cap L^2_{\rm loc}(0,+\infty;\boldsymbol{H}^1(\Omega)), \quad \boldsymbol{d} \in L^\infty(0,+\infty;\boldsymbol{H}^1(\Omega)).$$

Moreover,

$$\boldsymbol{d} \in L^2_{\rm loc}(0,+\infty;\boldsymbol{H}^2(\Omega)),$$

but this regularity is lost when $\varepsilon \to 0$.

On the other hand, this (GL) model verifies the *maximum principle's* result:

"If $|\boldsymbol{d}_0| \le 1$ in Ω and $|\boldsymbol{d}|_{\partial\Omega}| \le 1$ on $\partial\Omega \times (0,+\infty)$ (for the Dirichlet case), then $|\boldsymbol{d}| \le 1$ in Q". Finally, taking $\varepsilon \to 0$, one arrives at a limit $(\boldsymbol{u},\boldsymbol{d})$ which is a *measure-valued solution* of (EL), that is

$$\boldsymbol{u} \in L^\infty(0,+\infty;\boldsymbol{L}^2(\Omega)) \cap L^2_{\rm loc}(0,+\infty;\boldsymbol{H}^1(\Omega))), \quad \boldsymbol{d} \in L^\infty(0,+\infty;\boldsymbol{H}^1(\Omega)), \quad |\boldsymbol{d}| = 1 \ \text{ in } Q$$

and the elastic penalized tensor $(\nabla \boldsymbol{d}_\varepsilon)^t \nabla \boldsymbol{d}_\varepsilon$ goes to a measure $\mathcal{M}$ as $\varepsilon \to 0$.

Remark 4.1 *To identify $\mathcal{M}$ with $(\nabla \boldsymbol{d})^t \nabla \boldsymbol{d}$ is an interesting open problem.*

4.3 A generic second order scheme

During the last years many authors have focused their attention in designing and studying numerical schemes to approximate the problem (GL). For brevity in the notation, we consider a uniform partition of the time interval $[0,T]$, with $t^n = nk$ (where $k > 0$ denotes the fixed time step). Then, we write $(\boldsymbol{u}^n, p^n, \boldsymbol{d}^n, \boldsymbol{w}^n)$ as approximations of the exact solution at time t^n, $(\boldsymbol{u}(t^n), p(t^n), \boldsymbol{d}(t^n), \boldsymbol{w}(t^n))$, where $w = -\Delta \boldsymbol{d} + f_\varepsilon(\boldsymbol{d})$. By simplicity, we assume Neumann boundary conditions for $\boldsymbol{d}$: $\partial_{\boldsymbol{n}} \boldsymbol{d}(\boldsymbol{x},t) = 0$ on Σ.

We define the following numerical scheme, using a semi-implicit approximation in time: Given $(\boldsymbol{u}^n, \boldsymbol{d}^n)$, compute $(\boldsymbol{u}^{n+1}, p^{n+1}, \boldsymbol{d}^{n+1}, \boldsymbol{w}^{n+1}) \in \boldsymbol{U} \times P \times \boldsymbol{D} \times \boldsymbol{W}$ such that for any $(\bar{\boldsymbol{u}}, \bar{p}, \bar{\boldsymbol{d}}, \bar{\boldsymbol{w}}) \in \boldsymbol{U} \times P \times \boldsymbol{D} \times \boldsymbol{W}$:

$$\left\{\begin{array}{rcl} \big(\delta_t \boldsymbol{u}^{n+1}, \bar{\boldsymbol{u}}\big) + c(\widetilde{\boldsymbol{u}}, \boldsymbol{u}^{n+\frac12}, \bar{\boldsymbol{u}}) + \nu(\nabla \boldsymbol{u}^{n+\frac12}, \nabla \bar{\boldsymbol{u}}) & & \\ \qquad -(p^{n+\frac12}, \nabla\cdot \bar{\boldsymbol{u}}) - \lambda((\nabla \widetilde{\boldsymbol{d}})^t \boldsymbol{w}^{n+\frac12}, \bar{\boldsymbol{u}}) & = & 0 \\ (\nabla \cdot \boldsymbol{u}^{n+\frac12}, \bar{p}) & = & 0, \\ (\nabla \boldsymbol{d}^{n+\frac12}, \nabla \bar{\boldsymbol{d}}) + (\boldsymbol{f}^k_\varepsilon(\boldsymbol{d}^{n+1}, \boldsymbol{d}^n), \bar{\boldsymbol{d}}) - (\boldsymbol{w}^{n+\frac12}, \bar{\boldsymbol{d}}) & = & 0, \\ \big(\delta_t \boldsymbol{d}^{n+1}, \bar{\boldsymbol{w}}\big) + ((\boldsymbol{u}^{n+\frac12}\cdot\nabla)\widetilde{\boldsymbol{d}}, \bar{\boldsymbol{w}}) + \gamma(\boldsymbol{w}^{n+\frac12}, \bar{\boldsymbol{w}}) & = & 0, \end{array}\right. \tag{4.33}$$

where

$$c(\boldsymbol{u},\boldsymbol{v},\boldsymbol{w})=\Big(\boldsymbol{u}\cdot\nabla\boldsymbol{v},\boldsymbol{w}\Big)+\frac{1}{2}\Big((\nabla\cdot\boldsymbol{u})\boldsymbol{v},\boldsymbol{w}\Big). \tag{4.34}$$

Unknowns $\boldsymbol{w}^{n+\frac{1}{2}}$ and $p^{n+\frac{1}{2}}$ are approximations at midpoint $t^{n+\frac{1}{2}}:=(t^n+t^{n+1})/2$ (directly computed), while $\boldsymbol{u}^{n+\frac{1}{2}}:=(\boldsymbol{u}^{n+1}+\boldsymbol{u}^n)/2$ and $\boldsymbol{d}^{n+\frac{1}{2}}:=(\boldsymbol{d}^{n+1}+\boldsymbol{d}^n)/2$.

In order to obtain a second order in time scheme, we need to define $\boldsymbol{f}_\varepsilon^k(\boldsymbol{d}^{n+1},\boldsymbol{d}^n,\boldsymbol{d}^{n-1})$ as a second order approximation of $\boldsymbol{f}_\varepsilon^k(\boldsymbol{d}(t^{n+\frac{1}{2}}))$ and we also need to consider $\widetilde{\boldsymbol{u}}$ and $\widetilde{\boldsymbol{d}}$ as second order approximations of $\boldsymbol{u}(t_{n+\frac{1}{2}})$ and $\boldsymbol{d}(t_{n+\frac{1}{2}})$, respectively.

Testing in (4.33) by $(\bar{\boldsymbol{u}},\bar{p},\bar{\boldsymbol{d}},\bar{w})=(\boldsymbol{u}^{n+\frac{1}{2}},p^{n+\frac{1}{2}},\gamma\delta_t\boldsymbol{d}^{n+1},\gamma w^{n+\frac{1}{2}})$ and taking into account

$$c(\widetilde{\boldsymbol{u}},\boldsymbol{u}^{n+\frac{1}{2}},\boldsymbol{u}^{n+\frac{1}{2}})=0,$$

we obtain the following discrete energy law

$$\delta_t E_{tot}(\boldsymbol{u}^{n+1},\boldsymbol{d}^{n+1})+\nu\|\nabla\boldsymbol{u}^{n+\frac{1}{2}}\|^2_{L^2(\Omega)}+\lambda\gamma\|\boldsymbol{w}^{n+\frac{1}{2}}\|^2_{L^2(\Omega)}+\gamma ND_{phobic}(\boldsymbol{d}^{n+1},\boldsymbol{d}^n)=0 \tag{4.35}$$

where

$$\delta_t E_{tot}(\boldsymbol{u}^{n+1},\boldsymbol{d}^{n+1})=\frac{E_{tot}(\boldsymbol{u}^{n+1},\boldsymbol{d}^{n+1})-E_{tot}(\boldsymbol{u}^n,\boldsymbol{d}^n)}{k}.$$

and

$$ND_{phobic}(\boldsymbol{d}^{n+1},\boldsymbol{d}^n)=\int_\Omega \boldsymbol{f}_\varepsilon^k(\boldsymbol{d}^{n+1},\boldsymbol{d})\cdot\delta_t\boldsymbol{d}^{n+1}-\delta_t\left(\int_\Omega F_\varepsilon(\boldsymbol{d}^{n+1})\right).$$

Definition 4.2 *The numerical scheme* (4.35) *is energy-stable if it holds*

$$\delta_t E_{tot}(\boldsymbol{u}^{n+1},\boldsymbol{d}^{n+1})+\nu\|\nabla\boldsymbol{u}^{n+\frac{1}{2}}\|^2_{L^2(\Omega)}+\lambda\gamma\|\boldsymbol{w}^{n+\frac{1}{2}}\|^2_{L^2(\Omega)}\leq 0.$$

In particular, energy-stable schemes satisfy the energy decreasing in time property,

$$E_{tot}(\boldsymbol{u}^{n+1},\boldsymbol{d}^{n+1})\leq E_{tot}(\boldsymbol{u}^n,\boldsymbol{d}^n),\quad\forall\, n.$$

In particular, depending on the approximation considered of $\boldsymbol{f}_\varepsilon^k(\boldsymbol{d}^{n+1},\boldsymbol{d}^n)$ we will obtain different numerical schemes, with different discrete energy laws. In the following we summarize different numerical approximations of (GL) that have been presented in the literature in the last years using finite elements in space.

Remark 4.3 *Note that the last variational equality in (4.33) can be written as:*

$$\boldsymbol{w}^{n+\frac{1}{2}}=-\frac{1}{\gamma}P_{\boldsymbol{W}}^{L^2}\left(\delta_t\boldsymbol{d}^{n+1}+(\boldsymbol{u}^{n+\frac{1}{2}}\cdot\nabla)\tilde{\boldsymbol{d}}\right),$$

where $P_{\boldsymbol{W}}^{L^2}$ is the L^2-projector onto W. When a finite element approximation in space is considered, the following choices are possible (imposing in particular the inf-sup stability for velocity-pressure approximations):

- *$P_1+bubble/P_1$ or P_2/P_1 or P_2/P_0 for $(\boldsymbol{V}_h,P_h)\subset(\boldsymbol{H}_0^1(\Omega),L_0^2(\Omega))$,*
- *P_1/P_1 or P_2/P_2 or P_2/P_0 for $(\boldsymbol{D}_h,\boldsymbol{W}_h)\subset(\boldsymbol{H}^1(\Omega),\boldsymbol{L}^2(\Omega))$.*

In fact, the choice $\boldsymbol{W}_h=\boldsymbol{L}^2(\Omega)$ is also possible, see [56], and in this case the additional variable $\boldsymbol{w}$ is eliminated.

4.4 Some known numerical schemes

4.4.1 Lin-Liu approximation (LL)

In [55], the authors present a first order scheme where they decouple the fluid unknowns $(\boldsymbol{u}^{n+1}, p^{n+1})$ from the director vector $\boldsymbol{d}^{n+1}$. In particular, the potential term is approximated by the linear expression

$$\boldsymbol{f}_\varepsilon^k(\boldsymbol{d}^n, \boldsymbol{d}^{n+1}) = \frac{1}{\varepsilon^2}(|\boldsymbol{d}^n|^2\boldsymbol{d}^{n+1} - \boldsymbol{d}^{n+1}). \tag{4.36}$$

The unique solvability of the scheme can be assured by imposing the constraint $k < \varepsilon^2/\gamma$ but the energy-stability remains as an open problem.

4.4.2 Midpoint approximation (MP)

In [56], the additional variable $\boldsymbol{w}^{n+1}$ is eliminated rewritting the approximation of the non-gradient part of the elastic tensor $-\lambda((\nabla \boldsymbol{d}^n)^t\boldsymbol{w}, \bar{\boldsymbol{u}})$ by

$$\frac{\lambda}{\gamma}\left((\nabla \boldsymbol{d}^n)^t\left(\delta_t \boldsymbol{d}^{n+1} + (\boldsymbol{u}^{n+1}\cdot\nabla)\boldsymbol{d}^n\right), \bar{\boldsymbol{u}}\right).$$

Then, they combine this approach with the nonlinear midpoint (vectorial) approximation of the potential,

$$\boldsymbol{f}_\varepsilon^k(\boldsymbol{d}^{n+1}, \boldsymbol{d}^n) = \frac{F_\varepsilon(\boldsymbol{d}^{n+1}) - F_\varepsilon(\boldsymbol{d}^n)}{|\boldsymbol{d}^{n+1}|^2 - |\boldsymbol{d}^n|^2}(\boldsymbol{d}^{n+1} + \boldsymbol{d}^n). \tag{4.37}$$

In particular, this is a second order in time approximation of the potential and using the polynomial expression of $F_\varepsilon(\boldsymbol{d})$ one has

$$\boldsymbol{f}_\varepsilon^k(\boldsymbol{d}^{n+1}, \boldsymbol{d}^n) = \frac{1}{4\varepsilon^2}(|\boldsymbol{d}^{n+1}|^2 + |\boldsymbol{d}^n|^2 - 2)(\boldsymbol{d}^{n+1} + \boldsymbol{d}^n)$$

This scheme satisfies $ND_{phobic}(\boldsymbol{d}^{n+1}, \boldsymbol{d}^n) = 0$ and therefore it is unconditional energy-stable. Furthermore, following the ideas presented in [38] it is possible to assure the unique solvability of the scheme under the constraint $k < 2\varepsilon^2/\gamma$.

4.4.3 First order unconditionally stable approach (Eyre)

In [10], the authors present a nonlinear scheme whose approximation of the potential correspond with the extension of the ideas presented by Eyre in his celebrated preprint [29] but now in a vectorial framework. The idea is to split the potential into convex (+) and concave (-) part,

$$F_\varepsilon(\boldsymbol{d}) = F_+(\boldsymbol{d}) + F_-(\boldsymbol{d}) := \frac{1}{4\varepsilon^2}(|\boldsymbol{d}|^4 + 1) - \frac{1}{2\varepsilon^2}|\boldsymbol{d}|^2.$$

Taking the convex part in a implicit way and the concave part explicitly, the scheme satisfies $ND_{phobic}(\boldsymbol{d}^{n+1}, \boldsymbol{d}^n) \geq 0$ and then the unconditional energy-stability of the scheme is assured. In

particular, using polynomial expressions of $F_+(\boldsymbol{d})$ and $F_-(\boldsymbol{d})$, the nonlinear approximation of the potential term reads,

$$\boldsymbol{f}_\varepsilon^k(\boldsymbol{d}^{n+1},\boldsymbol{d}^n) = \nabla_{\boldsymbol{d}} F_+(\boldsymbol{d}^{n+1}) + \nabla_{\boldsymbol{d}} F_-(\boldsymbol{d}^n) = \frac{1}{\varepsilon^2}(|\boldsymbol{d}^{n+1}|^2\boldsymbol{d}^{n+1} - \boldsymbol{d}^n). \tag{4.38}$$

The scheme obtained using this approximation of the potential is uniquely solvable. Furthermore, when a space discretization is considered (with h the mesh size) one has the convergence as $(k,h)\to 0$ towards the penalized model (GL), and then as $\varepsilon\to 0$ towards the Erickseen-Leslie model (EL).

4.4.4 Explicit truncate approximation (Exp)

In [36] the authors consider a explicit approximation of a truncated potential term

$$\boldsymbol{f}_\varepsilon^k(\boldsymbol{d}^{n+1},\boldsymbol{d}^n) = \widetilde{\boldsymbol{f}}_\varepsilon(\boldsymbol{d}^n) = \begin{cases} \dfrac{1}{\varepsilon^2}(|\boldsymbol{d}^n|^2-1)\boldsymbol{d}^n & \text{if } |\boldsymbol{d}^n|\le 1, \\ \dfrac{2}{\varepsilon^2}(|\boldsymbol{d}^n|-1)\dfrac{\boldsymbol{d}^n}{|\boldsymbol{d}^n|} & \text{if } |\boldsymbol{d}^n|>1 \end{cases} \tag{4.39}$$

The scheme obtained is linear and unique solvable. When a space discretization is considered (with h the mesh size), the energy-stability of the scheme can be assured under the following constraints:

$$\lim_{(h,k,\varepsilon)\to 0}\frac{k}{h\varepsilon^2} = 0 \quad \text{and} \quad \boldsymbol{D}_h \subset \boldsymbol{W}_h.$$

Moreover, one has the convergence as $(k,h,\varepsilon)\to 0$ towards the Erickseen-Leslie model (EL) under the additional constraint

$$\lim_{(h,\varepsilon)\to 0}\frac{h}{\varepsilon^2} = 0.$$

4.4.5 First order Lagrange multiplier scheme (LM1)

In [6] the authors introduced $r = (|\boldsymbol{d}|^2-1)/\varepsilon^2$ as an approximation of the Lagrange multiplier associated to the restriction $|\boldsymbol{d}|=1$, and then the Ginzburg-Landau function can be rewritten as

$$\boldsymbol{f}_\varepsilon(d) = r\,\boldsymbol{d}.$$

Therefore, using the time derivative of this relation, we can rewrite the equality $\varepsilon^2 r = (|\boldsymbol{d}|^2-1)$ as the initial-value problem:

$$\varepsilon^2\partial_t r = 2\boldsymbol{d}\cdot\partial_t\boldsymbol{d} \quad \text{in } (0,T), \qquad \varepsilon^2 r(0) = |\boldsymbol{d}(0)|^2 - 1.$$

Using these ideas the first order approximation of the $\boldsymbol{d}$-system reads:

$$\begin{cases} (\nabla\boldsymbol{d}^{n+1},\nabla\bar{\boldsymbol{d}}) + (r^{n+1}\cdot\boldsymbol{d}^n,\bar{\boldsymbol{d}}) - (\boldsymbol{w}^{n+1},\bar{\boldsymbol{d}}) = 0, \\ \dfrac{\varepsilon^2}{2}\left(\delta_t r^{n+1},\bar{r}\right) = \left(\boldsymbol{d}^n\cdot\delta_t\boldsymbol{d}^{n+1},\bar{r}\right) \end{cases} \tag{4.40}$$

The scheme obtained is uniquely solvable and unconditionally energy-stable with respect to the modified energy

$$\widetilde{E}_{tot}(\boldsymbol{u},\boldsymbol{d},q) = E_{kin}(\boldsymbol{u}) + E_{ela}(\boldsymbol{d}) + \widetilde{E}_{pen}(r) \quad \text{with} \quad \widetilde{E}_{pen}(r) = (\varepsilon^2/4)\|r\|_{L^2}^2. \tag{4.41}$$

4.5 Second order numerical approximations of the potential term

We now propose some new approximations for the potential term $\boldsymbol{f}_\varepsilon^k(\boldsymbol{d}^{n+1},\boldsymbol{d}^n)$ based on the ideas presented in Section 3 to approximate Cahn-Hilliard equation.

4.5.1 Second order Lagrange multiplier scheme (LM2)

It is possible to extend the ideas of the previous section to derive the following second order approximation of the $\boldsymbol{d}$-system $(4.33)_3$:

$$\begin{cases} (\nabla \boldsymbol{d}^{n+\frac{1}{2}}, \nabla \bar{\boldsymbol{d}}) + (r^{n+\frac{1}{2}}\widetilde{\boldsymbol{d}}, \bar{\boldsymbol{d}}) - (\boldsymbol{w}^{n+\frac{1}{2}}, \bar{\boldsymbol{d}}) = 0, \\ \dfrac{\varepsilon^2}{2}\left(\delta_t r^{n+1}, \bar{r}\right) = \left(\widetilde{\boldsymbol{d}} \cdot \delta_t \boldsymbol{d}^{n+1}, \bar{r}\right). \end{cases} \tag{4.42}$$

for each $(\bar{\boldsymbol{d}}, \bar{r})$, where $r^{n+\frac{1}{2}} = (r^{n+1} + r^n)/2$. The scheme obtained using these ideas is uniquely solvable and unconditionally energy-stable for the modified energy given in (4.41).

4.5.2 Optimal dissipation approximation (OD2)

To extend the ideas of the **(OD2)** approximation to the Nematic Liquid Crystals model, we need to extend the Hermite quadrature formula exact for $\mathbb{P}_1$,

$$\int_a^b g(s)ds = (b-a)g(a) + \frac{1}{2}(b-a)g'(a) + C(b-a)^3 g''(\xi)$$

to a vectorial form. For any $\boldsymbol{d}^{n+1}$ and $\boldsymbol{d}^n$,

$$\frac{F(\boldsymbol{d}^{n+1}) - F(\boldsymbol{d}^n)}{k} = \frac{1}{k}\int_0^1 \frac{d}{ds} F(\boldsymbol{d}^n + s(\boldsymbol{d}^{n+1} - \boldsymbol{d}^n))ds.$$

Then, combining both expressions for

$$g(s) = \frac{d}{ds}F(\boldsymbol{d}^n + s(\boldsymbol{d}^{n+1} - \boldsymbol{d}^n)) = \boldsymbol{f}_\varepsilon(\boldsymbol{d}^n + s(\boldsymbol{d}^{n+1} - \boldsymbol{d}^n)) \cdot (\boldsymbol{d}^{n+1} - \boldsymbol{d}^n),$$

since

$$g'(s) = \left(\nabla_{\boldsymbol{d}} \boldsymbol{f}_\varepsilon(\boldsymbol{d}^n + s(\boldsymbol{d}^{n+1} - \boldsymbol{d}^n))(\boldsymbol{d}^{n+1} - \boldsymbol{d}^n)\right) \cdot (\boldsymbol{d}^{n+1} - \boldsymbol{d}^n),$$

we can arrive at the following potential approximation:

$$\boldsymbol{f}_\varepsilon^k(\boldsymbol{d}^{n+1},\boldsymbol{d}^n) = \boldsymbol{f}_\varepsilon(\boldsymbol{d}^n) + \frac{1}{2}\nabla_{\boldsymbol{d}} \boldsymbol{f}_\varepsilon(\boldsymbol{d}^n)(\boldsymbol{d}^{n+1} - \boldsymbol{d}^n).$$

For the (vectorial) Ginzburg-Landau potential $\boldsymbol{f}_\varepsilon(\boldsymbol{d})$, this expression yields to:

$$\boldsymbol{f}_\varepsilon^k(\boldsymbol{d}^{n+1},\boldsymbol{d}^n)=\frac{1}{\varepsilon^2}\left[(\boldsymbol{d}^n\cdot\boldsymbol{d}^{n+1})\boldsymbol{d}^n+|\boldsymbol{d}^n|^2\frac{\boldsymbol{d}^{n+1}-\boldsymbol{d}^n}{2}-\frac{\boldsymbol{d}^{n+1}+\boldsymbol{d}^n}{2}\right]. \tag{4.43}$$

Using ideas from [38], the unique solvability of the scheme can be assured under the constraint $k<2\varepsilon^2/\gamma$.

4.5.3 (MP-BDF2)

The key point is again to split the potential between convex (+) and concave (-) part

$$F_\varepsilon(\boldsymbol{d})=F_+(\boldsymbol{d})+F_-(\boldsymbol{d})\quad\text{ with }\quad F_+(\boldsymbol{d})=\frac{1}{4\varepsilon^2}(|\boldsymbol{d}|^4+1)\quad\text{ and }\quad F_-(\boldsymbol{d})=-\frac{1}{2\varepsilon^2}|\boldsymbol{d}|^2$$

and consider a midpoint **(MP)** approximation of the convex part and a second order backward difference formula **(BDF2)** of the concave and quadratic part, i.e,

$$\boldsymbol{f}_\varepsilon^k(\boldsymbol{d}^{n+1},\boldsymbol{d}^n,\boldsymbol{d}^{n-1})=\frac{F_+(\boldsymbol{d}^{n+1})-F_+(\boldsymbol{d}^n)}{|\boldsymbol{d}^{n+1}|^2-|\boldsymbol{d}^n|^2}(\boldsymbol{d}^{n+1}+\boldsymbol{d}^n)+\frac{1}{2}\Big(3\nabla_{\boldsymbol{d}}F_-(\boldsymbol{d}^n)-\nabla_{\boldsymbol{d}}F_-(\boldsymbol{d}^{n-1})\Big).$$

In particular, using the polynomial expressions of F_+ and F_-, one has:

$$\boldsymbol{f}_\varepsilon^k(\boldsymbol{d}^{n+1},\boldsymbol{d}^n,\boldsymbol{d}^{n-1})=\frac{1}{4\varepsilon^2}(|\boldsymbol{d}^{n+1}|^2+|\boldsymbol{d}^n|^2)(\boldsymbol{d}^{n+1}+\boldsymbol{d}^n)-\frac{1}{2\varepsilon^2}(3\boldsymbol{d}^n-\boldsymbol{d}^{n-1}).$$

4.5.4 (OD2-BDF2)

The idea is to split again the potential between convex and non-convex part and consider **(OD2)** approximation of the convex part and a second order backward difference formula **(BDF2)** of the non-convex part, i.e,

$$\boldsymbol{f}_\varepsilon^k(\boldsymbol{d}^{n+1},\boldsymbol{d}^n,\boldsymbol{d}^{n-1})=\boldsymbol{f}_+(\boldsymbol{d}^n)+\frac{1}{2}\nabla_{\boldsymbol{d}}\boldsymbol{f}_+(\boldsymbol{d}^n)(\boldsymbol{d}^{n+1}-\boldsymbol{d}^n)+\frac{1}{2}\Big(3\nabla_{\boldsymbol{d}}F_-(\boldsymbol{d}^n)-\nabla_{\boldsymbol{d}}F_-(\boldsymbol{d}^{n-1})\Big).$$

where $\boldsymbol{f}_+(\boldsymbol{d})=\nabla_{\boldsymbol{d}}F_+(\boldsymbol{d})$. This scheme is unconditionally unique solvable, but finding hypothesis to assure the energy-stability of this scheme remains as an open problem.

5 Application to other energy-based models

In this section we present some other physically motivated models that are in some sense related with the Cahn-Hilliard equation and where the ideas summarized in this work should be taken into account to derive efficient numerical schemes.

We are aware that there are a big amount of related models, and it is not our intention to try to summarize all of them here. We will just introduce two different models, that in recent times have become of increasingly interest.

5.1 Two phase flows with different densities.

We summarize here the model presented in [4] that can be viewed like a thermodynamic consistent coupling between Navier-Stokes equation for fluids with different densities and the Cahn-Hilliard equation. Let $\Omega \subset \mathbb{R}^d$ $(d = 2, 3)$ be a bounded domain, occupied by a mixture of two immiscible and incompressible fluids with different (and constant) densities $\rho_1 > \rho_2 > 0$. We denote $Q = \Omega \times (0, +\infty)$ and we consider that there is a mixing interface of small thickness:

$$\begin{cases} \rho \boldsymbol{u}_t + \Big((\rho \boldsymbol{u} + \boldsymbol{J}) \cdot \nabla\Big)\boldsymbol{u} - \nabla \cdot (2\eta(\phi)\boldsymbol{D}\boldsymbol{u}) + \nabla p + \lambda\varepsilon \nabla \cdot (\nabla\phi \otimes \nabla\phi) = 0, \\ \nabla \cdot \boldsymbol{u} = 0, \\ \rho_t + \nabla \cdot \Big(\rho \boldsymbol{u} + \boldsymbol{J}\Big) = 0, \\ \phi_t + \boldsymbol{u} \cdot \nabla\phi - \nabla \cdot (m(\phi)\nabla w) = 0, \\ -\lambda\varepsilon\Delta\phi + \dfrac{\lambda}{\varepsilon} f(\phi) = w. \end{cases} \tag{5.44}$$

Here $\boldsymbol{u}$ represents the mean velocity, p the pressure and ρ the density of the mixture, while ϕ is an order parameter (related to the difference of the volume fraction of each fluid) and w is the so-called chemical potential. Moreover, $\eta(\phi) > 0$ is the viscosity of the mixture (depending on the phase), λ is a constant related to the surface energy density, $\varepsilon > 0$ is a (small) parameter related to the thickness of the interface between the two fluids and $\boldsymbol{D}\boldsymbol{u} = \frac{1}{2}(\nabla \boldsymbol{u} + \nabla \boldsymbol{u}^t)$.

On the other hand, $m(\phi) > 0$ is the mobility function, $f(\phi) = F'(\phi)$ with $F(\phi)$ the polynomical double-well potential $F(\phi) = (\phi^2 - 1)^2/4$, and

$$\boldsymbol{J} = \frac{\rho_1 - \rho_2}{2} m(\phi)\nabla w$$

is a relative flux related to the diffusion of the components. Since $\rho_1 - \rho_2 > 0$, density moves from low to high concentration of the chemical potential w. This relative flux vanishes in the case of matched densities $\rho = \rho_2 = \rho_1 = const.$

Note that, taking into account ϕ-equation $(5.44)_4$, then ρ-equation $(5.44)_3$ is equivalent to the explicit relation

$$\rho(\phi) = \frac{\rho_1 + \rho_2}{2} + \frac{\rho_1 - \rho_2}{2}\phi := \rho_{med} + \rho_{dif}\phi. \tag{5.45}$$

The PDE system (5.44) is supplemented with the following initial and boundary conditions:

$$\boldsymbol{u}|_{t=0} = \boldsymbol{u}_0, \quad \phi|_{t=0} = \phi_0 \quad \text{in } \Omega,$$

$$\boldsymbol{u}|_{\partial\Omega} = 0, \quad \frac{\partial\phi}{\partial n}\Big|_{\partial\Omega} = 0, \quad \frac{\partial w}{\partial n}\Big|_{\partial\Omega} = 0 \quad \text{in } (0, T).$$

Under this assumptions the following (dissipative) energy law holds:

$$\frac{d}{dt}\int_\Omega \left(\rho(\phi)\frac{|\boldsymbol{u}|^2}{2} + \frac{\lambda\varepsilon}{2}|\nabla\phi|^2 + \frac{\lambda}{\varepsilon}F(\phi)\right)dx + 2\int_\Omega \eta(\phi)|\boldsymbol{D}\boldsymbol{u}|^2 dx + \int_\Omega m(\phi)|\nabla w|^2 dx = 0. \tag{5.46}$$

In particular, this energy law implies the dissipative character of the free energy

$$E(\boldsymbol{u},\phi)=\int_\Omega \rho(\phi)\frac{|\boldsymbol{u}|^2}{2}+\frac{\lambda\varepsilon}{2}\int_\Omega|\nabla\phi|^2+\frac{\lambda}{\varepsilon}\int_\Omega F(\phi)dx,$$

which is sum of the kinetic energy, the philic energy and the phobic one, respectively.

In order to define numerical schemes to approximate system (5.44), one should focus on schemes that are efficient in time and that satisfies a discrete version of the energy law (5.46). Indeed, in [39] a splitting numerical scheme that segregates the fluid part from the phase field part in a linear an energy-stable way has been derived. In that work, it is shown that it is possible to arrive to the following weak formulation:
Find (u,p,ϕ,w) such that

$$\begin{aligned}&\boldsymbol{u}\in L^\infty(0,T;\boldsymbol{L}^2(\Omega))\cap L^2(0,T;\boldsymbol{H}^1_0(\Omega)),\\&\phi\in L^\infty(0,T;H^1(\Omega)),\quad w\in L^2(0,T;H^1(\Omega)),\end{aligned}\tag{5.47}$$

and satisfying

$$\left\{\begin{array}{rcl}\Big(\rho(\phi)\boldsymbol{u}_t,\bar{\boldsymbol{u}}\Big)+\Big([(\rho(\phi)\boldsymbol{u}+\rho_{dif}m(\phi)\nabla w)\cdot\nabla]\boldsymbol{u},\bar{\boldsymbol{u}}\Big)&&\\ +2\Big(\eta(\phi)\boldsymbol{D}\boldsymbol{u},\boldsymbol{D}\bar{\boldsymbol{u}}\Big)-\Big(p,\nabla\cdot\bar{\boldsymbol{u}}\Big)+\Big(\phi\nabla w,\bar{\boldsymbol{u}}\Big)&=&0,\\ \Big(\nabla\cdot\boldsymbol{u},\bar{p}\Big)&=&0,\\ \Big(\phi_t,\bar{w}\Big)-\Big(\boldsymbol{u}\,\phi,\nabla\bar{w}\Big)+\Big(m(\phi)\nabla w,\nabla\bar{w}\Big)&=&0,\\ \lambda\varepsilon\Big(\nabla\phi,\nabla\bar{\phi}\Big)+\frac{\lambda}{\varepsilon}\Big(f(\phi),\bar{\phi}\Big)-\Big(w,\bar{\phi}\Big)&=&0,\end{array}\right.\tag{5.48}$$

for each $(\bar{\boldsymbol{u}},\bar{p},\bar{w},\bar{\phi})\in\boldsymbol{H}^1_0(\Omega)\times L^2_0(\Omega)\times H^1(\Omega)\times H^1(\Omega)$.

Using the ideas presented in the previous sections, it is possible to develop a generic first order scheme to approximate (5.48). For brevity in the notation, we consider a uniform partition of the time interval $[0,T]$, with $t^n=nk$ (where $k>0$ denotes the fixed time step). Then, we write $(\boldsymbol{u}^n,p^n,\phi^n,w^n)$ as approximations of the exact solution at time t^n, $(\boldsymbol{u}(t^n),p(t^n),\phi(t^n),w(t^n))$.

We define the following nonlinear numerical scheme, using an implicit-explicit approximation in time:
Given $(\boldsymbol{u}^n,\phi^n)$, compute $(\boldsymbol{u}^{n+1},p^{n+1},\phi^{n+1},w^{n+1})\in\boldsymbol{U}\times P\times V\times W$ such that for any $(\bar{\boldsymbol{u}},\bar{p},\bar{\phi},\bar{w})\in$

$\boldsymbol{U}\times P\times V\times W$:

$$\left\{\begin{array}{rcl}\Big(\rho([\phi^n])\delta_t\boldsymbol{u}^{n+1},\bar{\boldsymbol{u}}\Big)+\frac{1}{2}\Big(\boldsymbol{u}^{n+1}\delta_t\rho([\phi^{n+1}]),\bar{\boldsymbol{u}}\Big)&&\\ +\Big([(\rho(\phi^n)\boldsymbol{u}^n+\rho_{dif}m(\phi^n)\nabla w^{n+1})\cdot\nabla]\boldsymbol{u}^{n+1},\bar{\boldsymbol{u}}\Big)&&\\ +2\Big(\eta(\phi^n)\boldsymbol{D}\boldsymbol{u}^{n+1},\boldsymbol{D}\bar{\boldsymbol{u}}\Big)-\Big(p^{n+1},\nabla\cdot\bar{\boldsymbol{u}}\Big)+\Big(\phi^n\nabla w^{n+1},\bar{\boldsymbol{u}}\Big)&=&0,\\ \Big(\nabla\cdot\boldsymbol{u}^{n+1},\bar{p}\Big)&=&0,\\ \Big(\delta_t\phi^{n+1},\bar{w}\Big)-\Big(\boldsymbol{u}^{n+1}\,\phi^n,\nabla\bar{w}\Big)+\Big(m(\phi^n)\nabla w^{n+1},\nabla\bar{w}\Big)&=&0,\\ \lambda\varepsilon\Big(\nabla\phi^{n+1},\nabla\bar{\phi}\Big)+\frac{\lambda}{\varepsilon}\Big(f^k(\phi^{n+1},\phi^n),\bar{\phi}\Big)-\Big(w^{n+1},\bar{\phi}\Big)&=&0.\end{array}\right. \tag{5.49}$$

Theorem 5.1 *Scheme* (5.49) *is conservative because* $\int_\Omega\delta_t\phi^{n+1}=0$*, and it is energy-stable, in the sense that it satisfies the following discrete energy law:*

$$\begin{aligned}\frac{d}{dt}\int_\Omega\left(\rho(\phi^{n+1})\frac{|\boldsymbol{u}^{n+1}|^2}{2}+\frac{\lambda\varepsilon}{2}|\nabla\phi^{n+1}|^2+\frac{\lambda}{\varepsilon}F(\phi^{n+1})\right)dx+2\int_\Omega\eta(\phi^n)|\boldsymbol{D}\boldsymbol{u}^{n+1}|^2dx\\ +\int_\Omega m(\phi^n)|\nabla w^{n+1}|^2dx+ND^{n+1}_{philic}+\frac{\lambda}{\varepsilon}ND^{n+1}_{phobic}=0.\end{aligned} \tag{5.50}$$

where ND^{n+1}_{phobic} *is defined as in* (2.9) *and*

$$ND^{n+1}_{philic}=\frac{1}{2k}\|\nabla(\phi^{n+1}-\phi^n)\|^2_{L^2}+\frac{1}{2k}\int_\Omega\rho(\phi^n)|\boldsymbol{u}^{n+1}-\boldsymbol{u}^n|^2dx.$$

Remark 5.2 *Scheme* (5.49) *is energy-stable but it is nonlinear, and iterative algorithms have to be considered in order to approximate the system. In [39], a energy-stable linear scheme to approximate this model is presented.*

5.2 Vesicle Membranes

Vesicle Membranes are formed by certain amphi-philic molecules assembled in water to build bilayers. The molecules in the fluid-like membrane are free to wander and are allowed to shear at no cost. The bilayer structure makes Vesicle Membranes simple models for studying the physico-chemical properties of cell as well as of their shape deformations. Many works related with this topic has been introduced in the literature is the last years, focusing on the derivation of models [17, 18], establishment of analytical results of the systems [16, 21, 23] and their numerical approximations [19, 22].

In particular, we recall here the model derived in [17] to approximate the deformation of the fluid bound vesicle by means of an incompressible flow and phase field coupling. Indeed, this system can be viewed as a coupling between the Navier-Stokes equation with an Allen-Cahn system but where the energy related with the phase field function is the so-called bending energy and it is not the same energy considered in (1.1).

The phase function $\phi(x)$ plays the role of localizing the inside and the outside of the vesicle. We visualize that the level set $\{x : \phi(x) = 0\}$ gives the membrane, while $\{x : \phi(x) = 1\}$ represents the inside of the membrane and $\{x : \phi(x) = -1\}$ the outside. The corresponding interface motion is derived through the dynamics of this phase function by the energetic variational approach with respect to the bending energy associated to this phase field function. In particular, the bending energy is defined by the following expression:

$$E_\varepsilon(\phi) = \frac{1}{2\varepsilon}\int_\Omega \left[\varepsilon\Delta\phi - \frac{1}{\varepsilon}f(\phi)\right]^2 dx = \frac{1}{2\varepsilon}\int_\Omega \omega^2 dx \tag{5.51}$$

where

$$\omega = \varepsilon\Delta\phi - \frac{1}{\varepsilon}f(\phi). \tag{5.52}$$

The vesicle volume and surface area are approximated by

$$A(\phi) = \int_\Omega \phi\, dx \quad \text{and} \quad B(\phi) = \int_\Omega \left(\frac{\varepsilon}{2}|\nabla\phi|^2 + \frac{1}{\varepsilon}F(\phi)\right) dx, \tag{5.53}$$

respectively. The hydrodynamical system to study the vesicle deformation under external fields is derived from the total energy,

$$E_{tot}(\boldsymbol{u},\omega) = E_{kin}(\boldsymbol{u}) + E_\varepsilon(\omega) = \frac{1}{2}\int_\Omega |\boldsymbol{u}|^2 dx + \frac{1}{2\varepsilon}\int_\Omega \omega^2 dx. \tag{5.54}$$

In general, the system reads,

$$\begin{cases} \boldsymbol{u}_t - \nu\Delta\boldsymbol{u} + (\boldsymbol{u}\cdot\nabla)\boldsymbol{u} + \nabla p - \lambda\nabla\phi\left(\dfrac{\delta E_\varepsilon}{\delta\phi}\right) &= 0, \\ \nabla\cdot\boldsymbol{u} &= 0, \\ \phi_t + \boldsymbol{u}\cdot\nabla\phi + \gamma\left(\dfrac{\delta E_\varepsilon}{\delta\phi}\right) &= 0, \end{cases} \tag{5.55}$$

where

$$\frac{\delta E_\varepsilon}{\delta\phi} = -\Delta\omega + \frac{1}{\varepsilon^2}f'(\phi)\omega.$$

In particular, this system satisfies a dissipative energy law,

$$\delta_t E_{tot}(\boldsymbol{u},\omega) + \nu\|\nabla\boldsymbol{u}\|^2_{L^2(\Omega)} + \lambda\gamma\left\|\frac{\delta E_\varepsilon}{\delta\phi}\right\|^2_{L^2(\Omega)} = 0. \tag{5.56}$$

Due to the fact that the volume and the surface area of the vesicles have to remain constant in time, it is necessary to take into account how to enforce these two constraints while the numerical schemes are developed. Furthermore, one should design numerical schemes that satisfies discrete versions of the energy equality (5.56).

Denoting by $z = \dfrac{\delta E_\varepsilon}{\delta\phi}$, and taking the time derivative of equality (5.52) it is possible to arrive to the following weak formulation:

Find (u, p, ϕ, w, z) such that

$$\begin{aligned} &\boldsymbol{u} \in L^\infty(0,T;\boldsymbol{L}^2(\Omega)) \cap L^2(0,T;\boldsymbol{H}_0^1(\Omega)), \\ &\phi \in L^\infty(0,T;H^1(\Omega)), \quad w \in L^\infty(0,T;H^1(\Omega)), \quad z \in L^2(0,T;H^1(\Omega)), \end{aligned} \tag{5.57}$$

and satisfying

$$\left\{ \begin{array}{rcl} \langle \boldsymbol{u}_t, \bar{\boldsymbol{u}} \rangle + (\nu \nabla \boldsymbol{u}, \nabla \bar{\boldsymbol{u}}) + \Big((\boldsymbol{u} \cdot \nabla)\boldsymbol{u}, \bar{\boldsymbol{u}} \Big) + (\nabla p, \bar{u}) - \lambda (z \nabla \phi, \bar{\boldsymbol{u}}) &=& 0, \\ (\nabla \cdot \boldsymbol{u}, \bar{p}) &=& 0, \\ \langle \phi_t, \bar{z} \rangle + (\boldsymbol{u} \cdot \nabla \phi, \bar{z}) + \gamma (z, \bar{z}) &=& 0, \\ (\nabla \omega, \nabla \bar{\phi}) + \dfrac{1}{\varepsilon^2} (f'(\phi)\omega, \bar{\phi}) - (z, \bar{\phi}) &=& 0, \\ \dfrac{1}{\varepsilon} \langle \omega_t, \bar{\omega} \rangle - (\nabla \phi_t, \bar{\omega}) - \dfrac{1}{\varepsilon^2} (f'(\phi)\phi_t, \bar{\omega}) &=& 0, \end{array} \right. \tag{5.58}$$

for each $(\bar{\boldsymbol{u}}, \bar{p}, \bar{\phi}, \bar{\omega}, \bar{z}) \in \boldsymbol{H}_0^1(\Omega) \times L_0^2(\Omega) \times H^1(\Omega) \times H^1(\Omega) \times H^1(\Omega)$.

We define the following numerical scheme, using an implicit-explicit approximation in time: Given $(\boldsymbol{u}^n, \phi^n)$, compute $(\boldsymbol{u}^{n+1}, p^{n+1}, \phi^{n+1}, w^{n+1}, z^{n+1}) \in \boldsymbol{U} \times P \times V \times W \times Z$ such that for any $(\bar{\boldsymbol{u}}, \bar{p}, \bar{\phi}, \bar{w}, \bar{z}) \in \boldsymbol{U} \times P \times V \times W \times Z$:

$$\left\{ \begin{array}{rcl} \big(\delta_t \boldsymbol{u}^{n+1}, \bar{\boldsymbol{u}} \big) + (\nu \nabla \boldsymbol{u}^{n+1}, \nabla \bar{\boldsymbol{u}}) + c(\boldsymbol{u}^n, \boldsymbol{u}^{n+1}, \bar{\boldsymbol{u}}) + (\nabla p^{n+1}, \bar{u}) - \lambda (z^{n+1} \nabla \phi^n, \bar{\boldsymbol{u}}) &=& 0, \\ (\nabla \cdot \boldsymbol{u}^{n+1}, \bar{p}) &=& 0, \\ \big(\delta_t \phi^{n+1}, \bar{z} \big) + (\boldsymbol{u}^{n+1} \cdot \nabla \phi^n, \bar{z}) + \gamma (z^{n+1}, \bar{z}) &=& 0, \\ (\nabla \omega^{n+1}, \nabla \bar{\phi}) + \dfrac{1}{\varepsilon^2} (f'(\phi^n)\omega^{n+1}, \bar{\phi}) - (z^{n+1}, \bar{\phi}) &=& 0, \\ \dfrac{1}{\varepsilon} (\delta_t \omega^{n+1}, \bar{\omega}) - (\nabla \delta_t (\phi^{n+1}), \nabla \bar{\omega}) - \dfrac{1}{\varepsilon^2} (f'(\phi^n)\delta_t \phi^{n+1}, \bar{\omega}) &=& 0, \end{array} \right. \tag{5.59}$$

where $c(\boldsymbol{u}^n, \boldsymbol{u}^{n+1}, \bar{\boldsymbol{u}})$ is defined as in (4.34).

Theorem 5.3 *Scheme* (5.59) *is energy-stable in the sense that the following discrete energy law holds:*

$$\delta_t E_{tot}(\boldsymbol{u}^{n+1}, \omega^{n+1}) + \nu \|\nabla \boldsymbol{u}^{n+1}\|_{L^2(\Omega)}^2 + \lambda\gamma \left\| z^{n+1} \right\|_{L^2(\Omega)}^2 + ND^{n+1} = 0, \tag{5.60}$$

where the numerical dissipation reads

$$ND^{n+1} = \frac{1}{k} \|\boldsymbol{u}^{n+1} - \boldsymbol{u}^n\|_{L^2}^2 + \frac{1}{k\,\varepsilon} \|\omega^{n+1} - \omega^n\|_{L^2}^2.$$

Remark 5.4 *Scheme* (5.59) *is energy-stable but the constraints of conservation of volume and surface do not hold. Derive efficient energy-stable schemes satisfying the physical constraints remains as an open problem.*

6 Conclusions

In this work, we have presented an overview of the different numerical schemes introduced in the literature to approximate the Cahn-Hilliard equation and some related models. The natural question that arises is: *"Which one is the optimal approach?"*. The answer to this question we dare not venture to report because it is not clear, it will depends on what do you expect from your numerical scheme. In Table 1 we outline the main properties of each of the schemes and we hope it can be used as a guide to the ones that have not already decided which approximation suits better with their desires.

	Linear	**Uncon. Solva**	**Uncon. Energy-Stable**	**One-Step Alg.**	$O(k^\alpha)$
E1	X	✓	✓	✓	1
MP	X	X	✓	✓	2
GH	X	?	✓	✓	2
TE	X	?	✓	✓	2
MP-BDF2	X	✓	✓*	X	2
EL1	✓	?	✓**	✓	1
OD2	✓	X	X	✓	2
OD2-BDF2	✓	✓	X	X	2
WVV	✓	X	✓**	✓	2
LM2	✓	✓	✓*	X	2

* for a modified energy $\tilde{E}(\phi)$.

** introducing enough amount of numerical dissipation and considering a modified potential $\tilde{F}(\phi)$.

Table 1: Features of schemes

We have also recalled in this work the great connection that the Cahn-Hilliard equation has with many other physically motivated models. Basically, all these models have in common that can be formulated starting from some energy. In particular, we have reviewed three different models: two fluid flows with different densities, Vesicle Membranes and Nematic Liquid Crystals. Indeed, in the case of the Nematic Liquid Crystals we have shown different numerical approximations that were introduced in the literature, showing a clear connection with the ideas presented in the Cahn-Hilliard framework.

Finally, we would like to mention that there are not too many results showing the convergence of the solutions of the numerical schemes to the solution of the original continuous problem, and maybe this crucial step will give some new insights to decide which of the numerical approximations is more convenient.

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